National Library of Medicine
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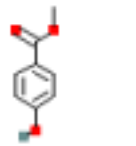
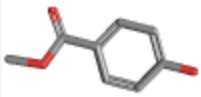
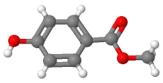
COMPOUND SUMMARY

Methylparaben

Cite Download

PubChem CID	7456
Structure	 2D  3D  Crystal
Chemical Safety	Irritant Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_8H_8O_3$
Synonyms	Methyl 4-hydroxybenzoate METHYLPARABEN 99-76-3 Methyl paraben Methyl p-hydroxybenzoate View More...
Molecular Weight	152.15 g/mol *Computed by PubChem 2.2 (PubChem release 2021.10.14)*
Dates	Create: 2005-03-26 Modify: 2024-04-06

Description

Methylparaben is a 4-hydroxybenzoate ester resulting from the formal condensation of the carboxy group of 4-hydroxybenzoic acid with methanol. It is the most frequently used antimicrobial preservative in cosmetics. It occurs naturally in several fruits, particularly in blueberries. It has a role as a plant metabolite, an antimicrobial food preservative, a neuroprotective agent and an antifungal agent.

▸ ChEBI

Methylparaben is used in allergenic testing.

▸ DrugBank

Methylparaben is a Standardized Chemical Allergen. The physiologic effect of methylparaben is by means of Increased Histamine Release, and Cell-mediated Immunity.

▸ FDA Pharm Classes

View More...

See also: Butylparaben; ethylparaben; methylparaben (component of) ... View More ...

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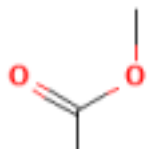
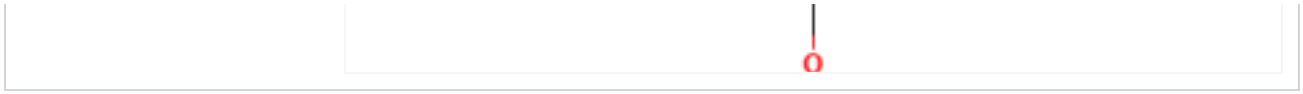
1 Structures

1.1 2D Structure

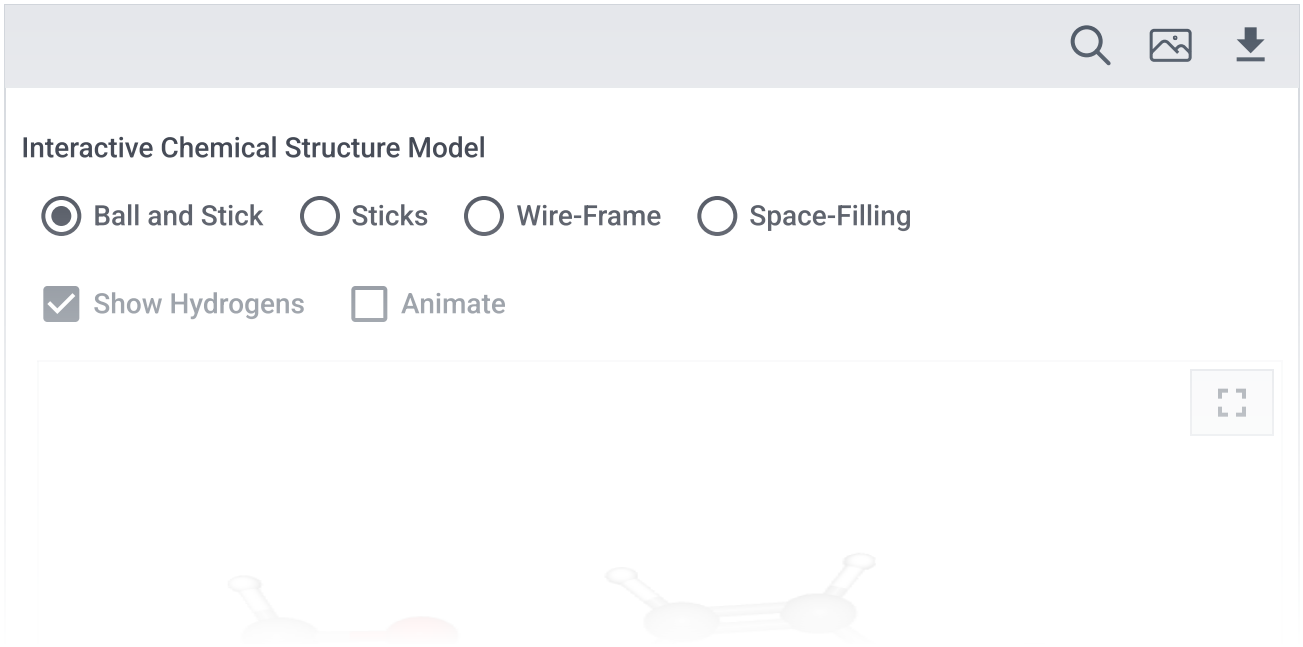
Chemical Structure Depiction





PubChem

1.2 3D Conformer

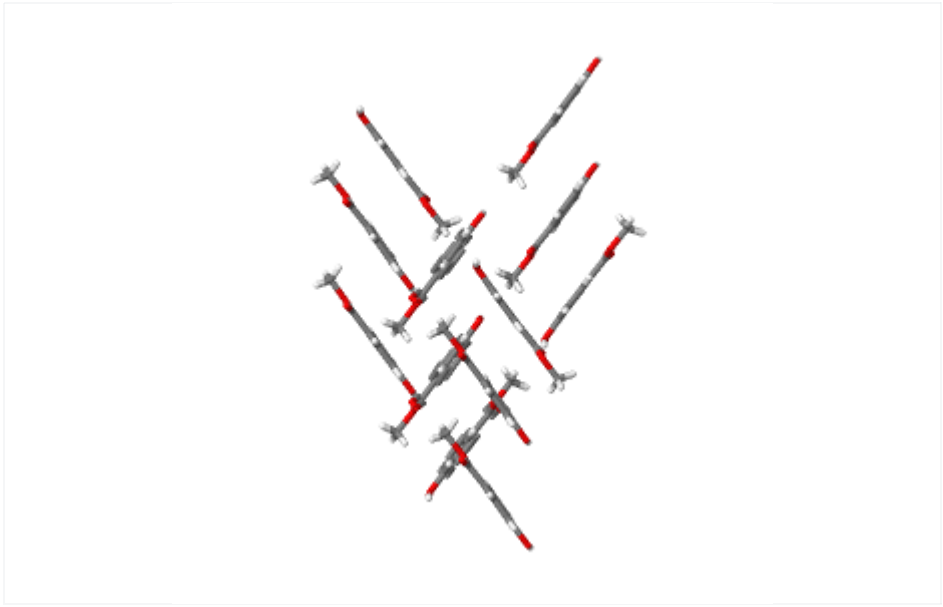


PubChem

1.3 Crystal Structures

1 of 11	View All
CCDC Number	617627
Associated Article	DOI:10.1021/cg050639k
Crystal Structure Data	DOI:10.5517/ccnqpgh

Crystal Structure Depiction



▸ The Cambridge Structural Database

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

methyl 4-hydroxybenzoate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.10.14)

▸ PubChem

2.1.2 InChI

InChI=1S/C8H8O3/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5,9H,1H3

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

▸ PubChem

2.1.3 InChIKey

LXCFILQKKLGQFO-UHFFFAOYSA-N

Computed by InChI 1.0.6 (PubChem release 2021.10.14)

PubChem

2.1.4 Canonical SMILES

COC(=O)C1=CC=C(C=C1)O

Computed by OEChem 2.3.0 (PubChem release 2021.10.14)

PubChem

2.2 Molecular Formula

$C_8H_8O_3$

Computed by PubChem 2.2 (PubChem release 2021.10.14)

EU Food Improvement Agents; PubChem

2.3 Other Identifiers

2.3.1 CAS

99-76-3

CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemical Data Reporting (CDR...

2.3.2 Related CAS

5026-62-0 (hydrochloride salt)

ChemIDplus

2.3.3 Deprecated CAS

1000398-37-7, 156291-94-0, 58339-84-7

ChemIDplus; EPA Chemicals under the TSCA

1000398-37-7, 58339-84-7

- EPA DSSTox

2.3.4 European Community (EC) Number

243-171-5

- EU Food Improvement Agents

202-785-7

- European Chemicals Agency (ECHA)

2.3.5 UNII

A2I8C7HI9T

- FDA Global Substance Registration System (GSRS)

2.3.6 ChEBI ID

CHEBI:31835

- ChEBI

2.3.7 ChEMBL ID

CHEMBL325372

- ChEMBL

2.3.8 DrugBank ID

DB14212

- DrugBank

2.3.9 DSSTox Substance ID

DTXSID4022529

- EPA DSSTox

2.3.10 FEMA Number

2710

- Flavor and Extract Manufacturers Association (FEMA)

2.3.11 HMDB ID

HMDB0032572

- Human Metabolome Database (HMDB)

2.3.12 KEGG ID

D01400

- KEGG

2.3.13 Metabolomics Workbench ID

45617

- Metabolomics Workbench

2.3.14 NCI Thesaurus Code

C76720

- NCI Thesaurus (NCIt)

2.3.15 Nikkaji Number

J3.996I

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.16 NSC Number

406127

- DTP/NCI

3827

- DTP/NCI

2.3.17 Pharos Ligand ID

AYT63ZDRP3G6

- Pharos

2.3.18 RXCUI

29903

- NLM RxNorm Terminology

2.3.19 Wikidata

Q229987

- Wikidata

2.3.20 Wikipedia

Methylparaben

- Wikipedia

2.4 Synonyms

2.4.1 MeSH Entry Terms

4-hydroxybenzoic acid methyl ester
methyl p-hydroxybenzoate
methyl-4-hydroxybenzoate
methylparaben
methylparaben, sodium salt
Nipagin

▸ Medical Subject Headings (MeSH)

2.4.2 Depositor-Supplied Synonyms

Methyl 4-hydroxybenzoate
METHYLPARABEN
99-76-3
Methyl paraben
Methyl p-hydroxybenzoate
Nipagin
Methyl parahydroxybenzoate
Tegosept M
Moldex
Maseptol
Preserval M
Methaben
Metoxyde
Preserval
Metaben
Paridol
Septos
Solbrol
Methyl butex
p-Hydroxybenzoic acid methyl ester
p-Methoxycarbonylphenol
Benzoic acid, 4-hydroxy-, methyl ester
Methyl chemosept
p-Carbomethoxyphenol
4-Hydroxybenzoic acid methyl
Methyl parasept
Nipagin M
Aseptoform
Methylben
Abiol
Methyl-p-hydroxybenzoate
Methyl p-oxybenzoate
Solbrol M

▸ PubChem

3 Chemical and Physical Properties

3.1 Computed Properties

Property Name	Property Value	Reference
Molecular Weight	152.15 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
XLogP3	2	Computed by XLogP3 3.0 (PubChem release 2021.10.14)

Property Name	Property Value	Reference
Hydrogen Bond Donor Count	1	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Hydrogen Bond Acceptor Count	3	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Rotatable Bond Count	2	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Exact Mass	152.047344113 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Monoisotopic Mass	152.047344113 g/mol	Computed by PubChem 2.2 (PubChem release 2021.10.14)
Topological Polar Surface Area	46.5Å²	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Heavy Atom Count	11	Computed by PubChem
Formal Charge	0	Computed by PubChem
Complexity	136	Computed by Cactvs 3.4.8.18 (PubChem release 2021.10.14)
Isotope Atom Count	0	Computed by PubChem
Defined Atom Stereocenter Count	0	Computed by PubChem
Undefined Atom Stereocenter Count	0	Computed by PubChem
Defined Bond Stereocenter Count	0	Computed by PubChem
Undefined Bond Stereocenter Count	0	Computed by PubChem
Covalently-Bonded Unit Count	1	Computed by PubChem
Compound Is Canonicalized	Yes	Computed by PubChem (release 2021.10.14)

▸ PubChem

3.2 Experimental Properties

3.2.1 Physical Description

Dry Powder

- EPA Chemical Data Reporting (CDR)

Almost odourless, small colourless crystals or white crystalline powder

- EU Food Improvement Agents

Colorless or white solid; [HSDB] White odorless powder; [MSDSonline]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Solid

- Human Metabolome Database (HMDB)

3.2.2 Color / Form

White needles

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1132

- Hazardous Substances Data Bank (HSDB)

Colorless crystals or white crystalline powder

Lewis, R.J. Sax's Dangerous Properties of Industrial Materials. 10th ed. Volumes 1-3 New York, NY: John Wiley & Sons Inc., 1999., p. V3: 2013

- Hazardous Substances Data Bank (HSDB)

Needles from dil alcohol

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-376

- Hazardous Substances Data Bank (HSDB)

3.2.3 Odor

Odorless or has faint characteristic odor

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 915

▸ Hazardous Substances Data Bank (HSDB)

3.2.4 Taste

Slight burning taste

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 915

▸ Hazardous Substances Data Bank (HSDB)

3.2.5 Boiling Point

270.5 °C (decomposes)

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-376

▸ Hazardous Substances Data Bank (HSDB)

275.00 °C. @ 760.00 mm Hg

The Good Scents Company Information System

▸ Human Metabolome Database (HMDB)

3.2.6 Melting Point

ofp-hydroxybenzoic acid derived from the sample is 213 °C to 217 °C after drying for two hours at 80 °C

▸ EU Food Improvement Agents

125.2 °C

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-376

▸ Hazardous Substances Data Bank (HSDB)

131 °C

- Human Metabolome Database (HMDB)

3.2.7 Solubility

In water, 2.50X10+3 mg/L at 25 °C

Yalkowsky, S.H., He, Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010, p. 481

- Hazardous Substances Data Bank (HSDB)

Solubility in water (w/w): 0.25% at 20 °C; 0.30% at 25 °C

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1132

- Hazardous Substances Data Bank (HSDB)

Solubilities in various solvents

Solvent	g/100g at 25 °C
Methanol	59
Ethanol	52
Propylene glycol	22
Peanut oil	0.5
Acetone	64
Benzene	0.7
Ether	23
Carbon tetrachloride	0.1

Thomas MR; Salicylic Acid and Related Compounds. Ullmann's Encyclopedia of Industrial Chemistry. 7th ed. (1999-2016). New York, NY: John Wiley & Sons. Online Posting Date: 26 Jan 2006.

- Hazardous Substances Data Bank (HSDB)

Slightyl soluble in water; very soluble in ethanol, ether, acetone; soluble in trfluoroacetic acid

Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton:

FL 2014-2015, p. 3-376

- Hazardous Substances Data Bank (HSDB)

For more Solubility (Complete) data for METHYLPARABEN (6 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

2.5 mg/mL at 25 °C

- Human Metabolome Database (HMDB)

3.2.8 Vapor Pressure

0.000237 [mmHg]

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.2.9 LogP

log Kow = 1.96

Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 42

- Hazardous Substances Data Bank (HSDB)

1.96

- Human Metabolome Database (HMDB)

3.2.10 Stability / Shelf Life

Stable under recommended storage conditions.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

- Hazardous Substances Data Bank (HSDB)

Parabens are stable against hydrolysis during autoclaving & resist saponification /

Parabens/

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 124

▸ Hazardous Substances Data Bank (HSDB)

Calcium salts /are/ stable; sodium salts /are/ unstable. /Parabens/

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 124

▸ Hazardous Substances Data Bank (HSDB)

3.2.11 Decomposition

When heated to decomp it emits acrid smoke and fumes.

Lewis, R.J. Sr. (ed) Sax's Dangerous Properties of Industrial Materials. 11th Edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. 2004., p. 2004

▸ Hazardous Substances Data Bank (HSDB)

3.2.12 Ionization Efficiency

Ionization mode	Positive
logIE	1.22
pH	2.7
Instrument	Agilent XCT
Ion source	Electrospray ionization
Additive	formic acid (5.3nM)
Organic modifier	MeCN (80%)
Reference	DOI:10.1038/s41598-020-62573-z

▸ Kruve Lab, Ionization & Mass Spectrometry, Stockholm University

3.2.13 Collision Cross Section

128.43 Å² $[M-H]^-$

126.1 Å² $[M+H]^+$

S61 | UJICCSLIB | Collision Cross Section (CCS) Library from UJI | DOI:10.5281/zenodo.3549476

▸ NORMAN Suspect List Exchange

3.2.14 Kovats Retention Index

Standard non-polar	1435, 1419, 1410, 1420, 1419, 1435, 1419
Semi-standard non-polar	1452, 1470.4, 1459, 1465, 1460, 1475
Standard polar	2932, 2930, 2932, 2911, 2925

▸ NIST Mass Spectrometry Data Center

3.2.15 Other Experimental Properties

When heated to decomposition, emits acrid smoke and fumes

David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2016). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012

▸ Hazardous Substances Data Bank (HSDB)

3.3 SpringerMaterials Properties

Boiling point
Chemical shift
Density
Diamagnetic susceptibility
Fusion temperature
Heat of sublimation
Lineshape
Magnetic susceptibility
Melting temperature
Optical coefficient
Phase transition
Refractive index
Surface tension
Transition enthalpy
Vapor pressure
Viscosity

- SpringerMaterials

3.4 Chemical Classes

Other Uses -> Preservatives

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

3.4.1 Food Additives

Food addtives -> FDA Substances Added to Food (formerly EAFUS)

- FDA Center for Food Safety and Applied Nutrition (CFSAN)

4 Spectral Information

4.1 1D NMR Spectra

1 of 2	
1D NMR Spectra	NMR: 1191 (Sadtler Research Laboratories Spectral Collection)

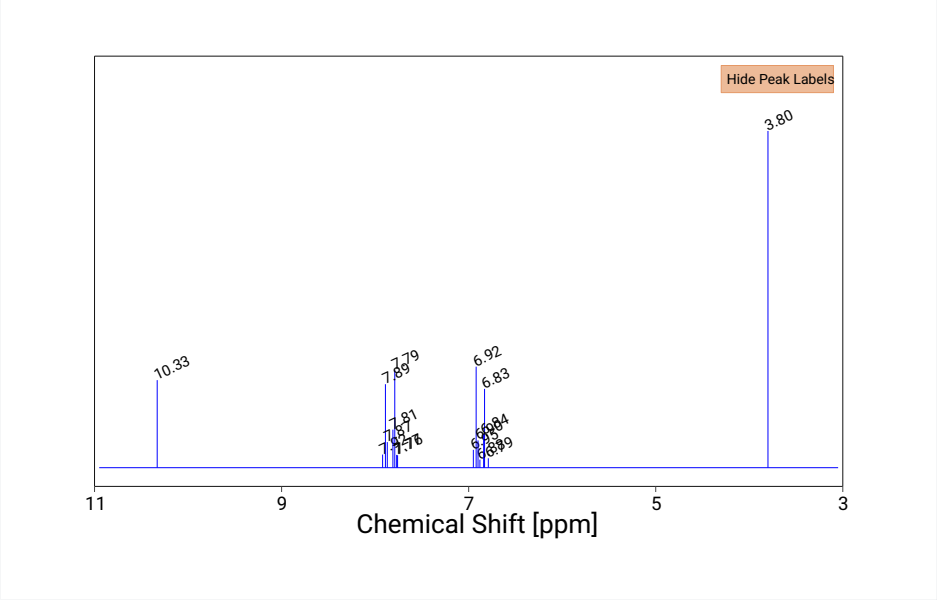
- Hazardous Substances Data Bank (HSDB)

2 of 2	
1D NMR Spectra	NMRShiftDB Link

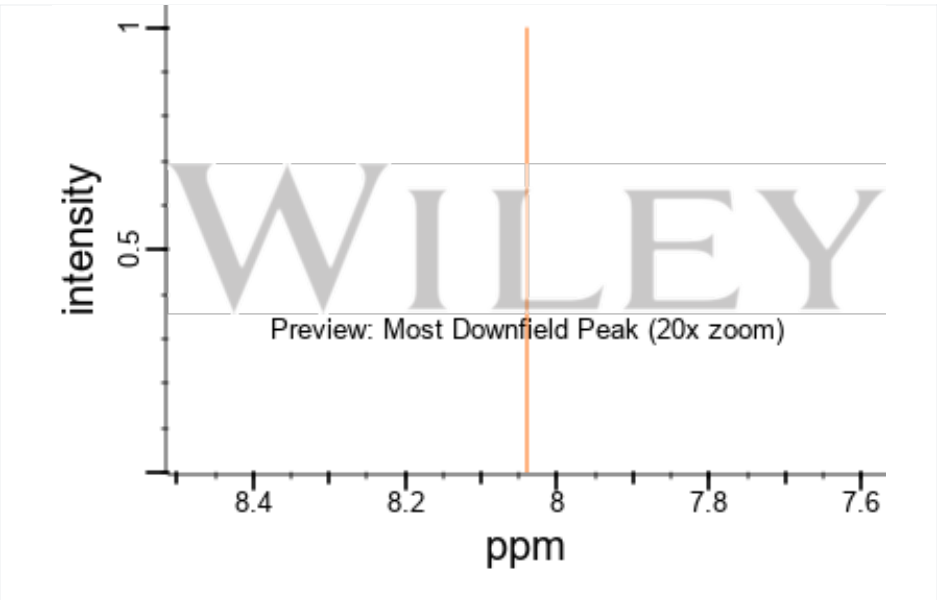
- NMRShiftDB

4.1.1 1H NMR Spectra

1 of 3	View All
Spectra ID	2746
Instrument Type	JEOL
Frequency	90 MHz

Solvent	DMSO-d6
Shifts [ppm]:Intensity	7.79:289.00, 3.80:1000.00, 6.83:234.00, 7.92:39.00, 6.92:300.00, 6.88:24.00, 7.77:38.00, 7.81:113.00, 6.95:53.00, 7.76:37.00, 7.89:248.00, 6.90:81.00, 6.79:28.00, 6.84:98.00, 7.87:76.00, 10.33:260.00
Thumbnail	

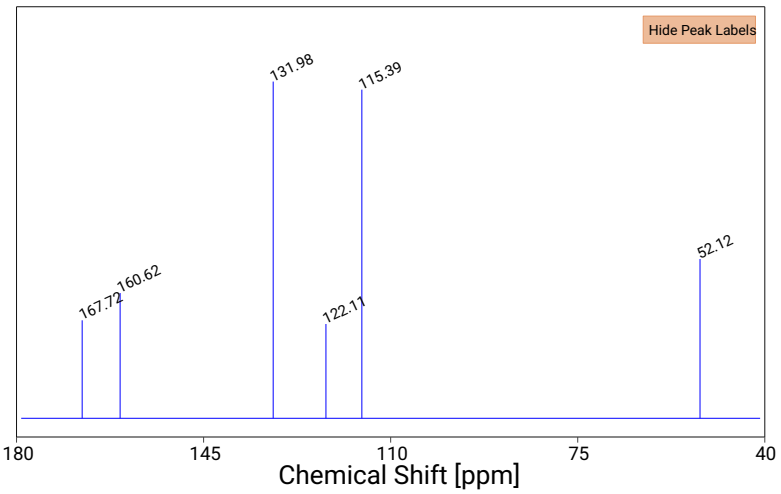
▸ Human Metabolome Database (HMDB)

2 of 3	View All
Instrument Name	Varian A-60
Source of Sample	Heyden-Newport Chemical Corporation, New York, New York
Copyright	Copyright © 2009-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

SpectraBase

4.1.2 13C NMR Spectra

1 of 3 View All

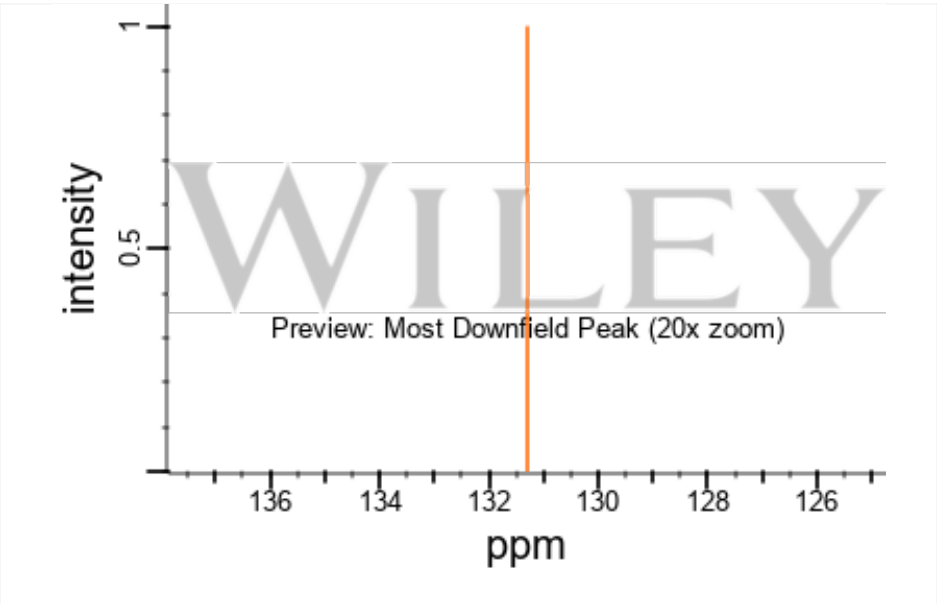
Spectra ID	3440
Frequency	50.18 MHz
Solvent	CDCl3
Shifts [ppm]:Intensity	115.39:976.00, 122.11:280.00, 131.98:1000.00, 160.62:372.00, 52.12:473.00, 167.72:291.00
Thumbnail	

Human Metabolome Database (HMDB)

2 of 3 View All

Source of Sample	E. Merck AG, Darmstadt, Germany
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



WILEY

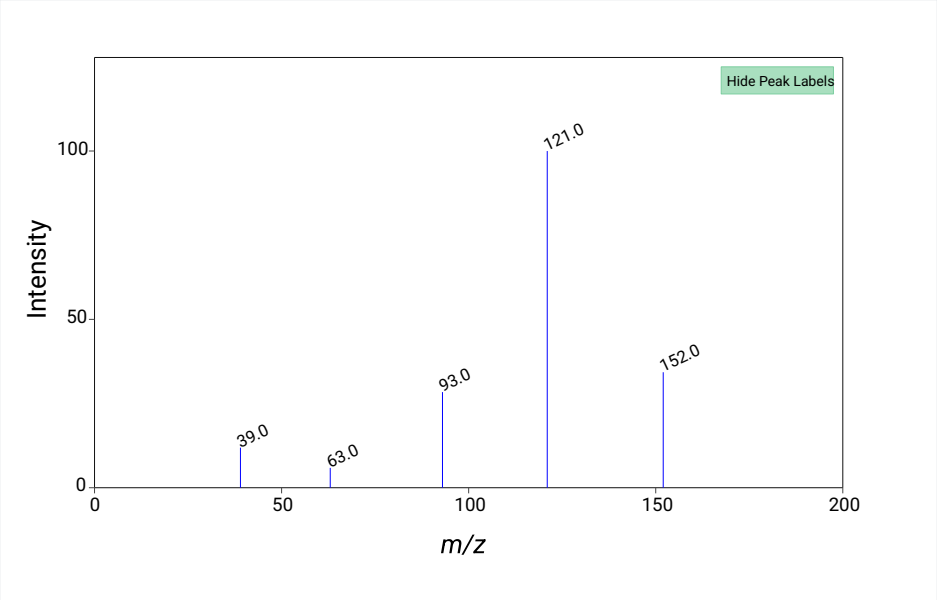
SpectraBase

4.2 Mass Spectrometry

4.2.1 GC-MS

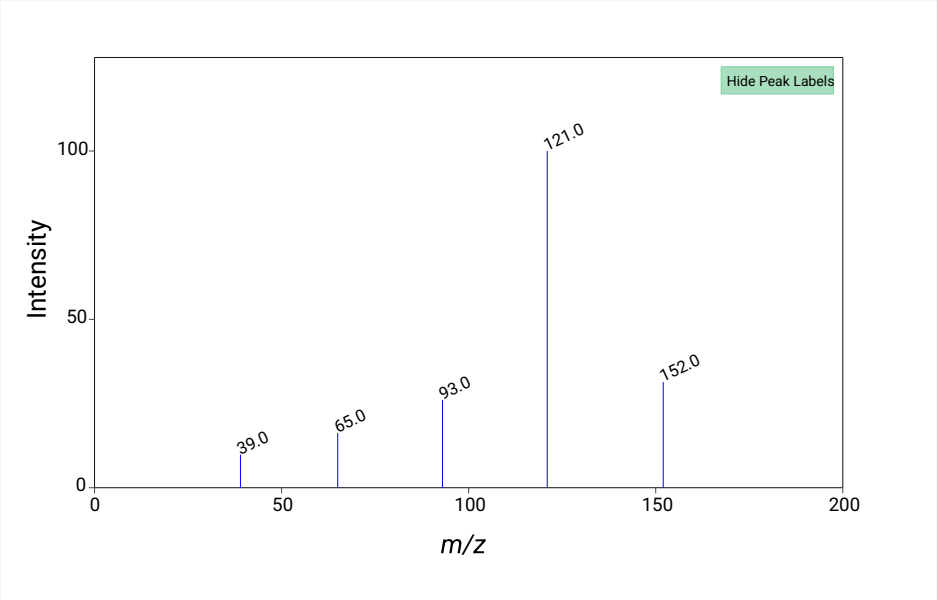
1 of 23 View All

Spectra ID	101182
Instrument Type	EI-B
Ionization Mode	positive
SPLASH	splash10-00di-4900000000-c5ef5603a5b5d1102f5a
Top 5 Peaks	121.0 99.99 152.0 34.30 93.0 28.40 39.0 11.90 63.0 5.90

Thumbnail	
Notes	instrument=SHIMADZU LKB-9000B

▸ Human Metabolome Database (HMDB)

2 of 23	View All
Spectra ID	26760
Instrument Type	EI-B
Ionization Mode	positive
SPLASH	splash10-00di-4900000000-5aa5692082b66b714b5d
Top 5 Peaks	121.0 99.99 152.0 31.38 93.0 26.08 65.0 16.25 39.0 9.82

Thumbnail	
Notes	instrument=HITACHI RMU-7M

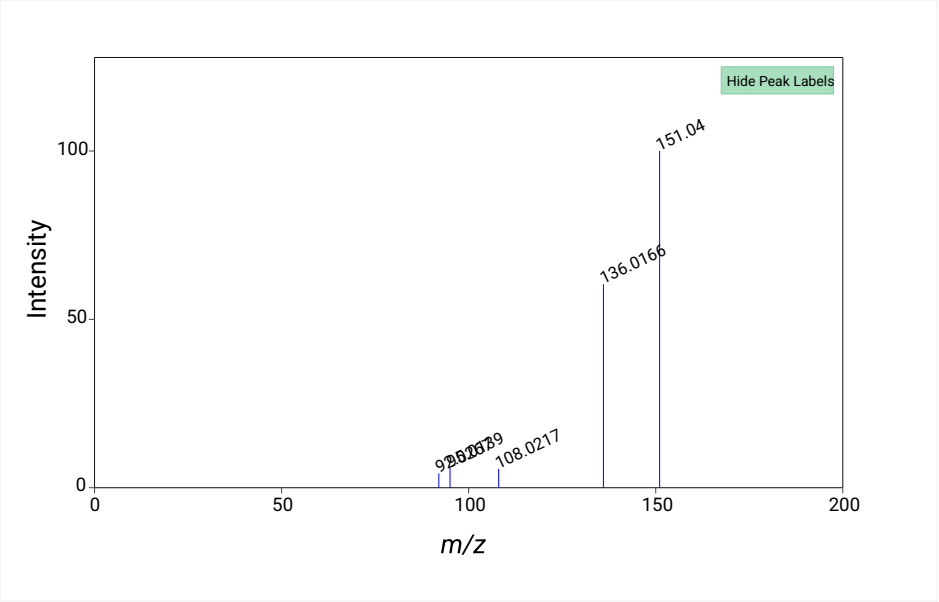
▸ Human Metabolome Database (HMDB)

4.2.2 MS-MS

1 of 7 View All

Spectra ID	2236662
Ionization Mode	Negative
SPLASH	splash10-0udr-0900000000-2e50ec52313e18cddbd0
Top 5 Peaks	151.04 100 136.0166 60.46 95.0139 5.91 108.0217 5.58 92.0267 4.25

Thumbnail

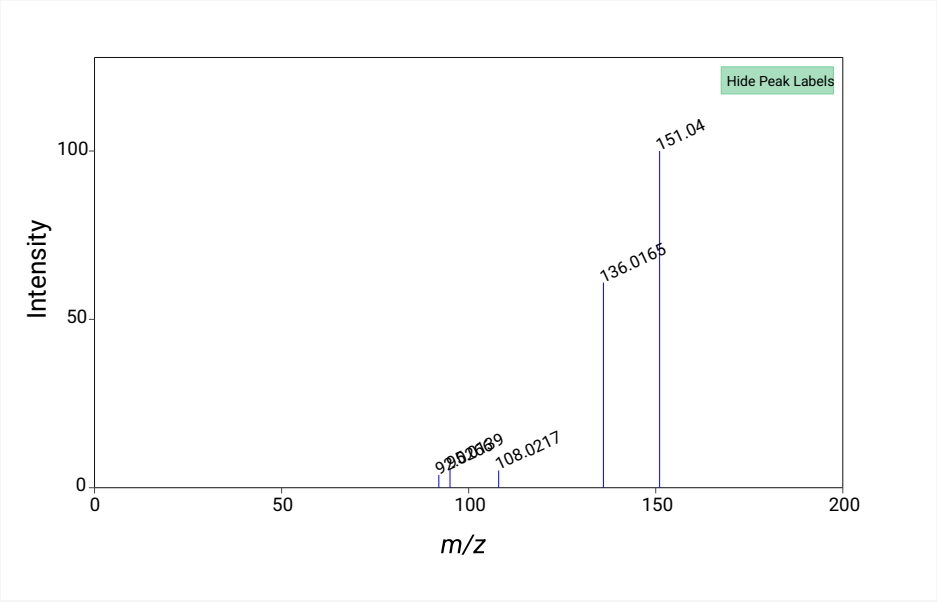


Human Metabolome Database (HMDB)

2 of 7 View All

Spectra ID	2236697
Ionization Mode	Negative
SPLASH	splash10-0udr-0900000000-10b0539cab1169d8d877
Top 5 Peaks	151.04 100 136.0165 60.93 95.0139 5.46 108.0217 5.13 92.0266 3.76

Thumbnail

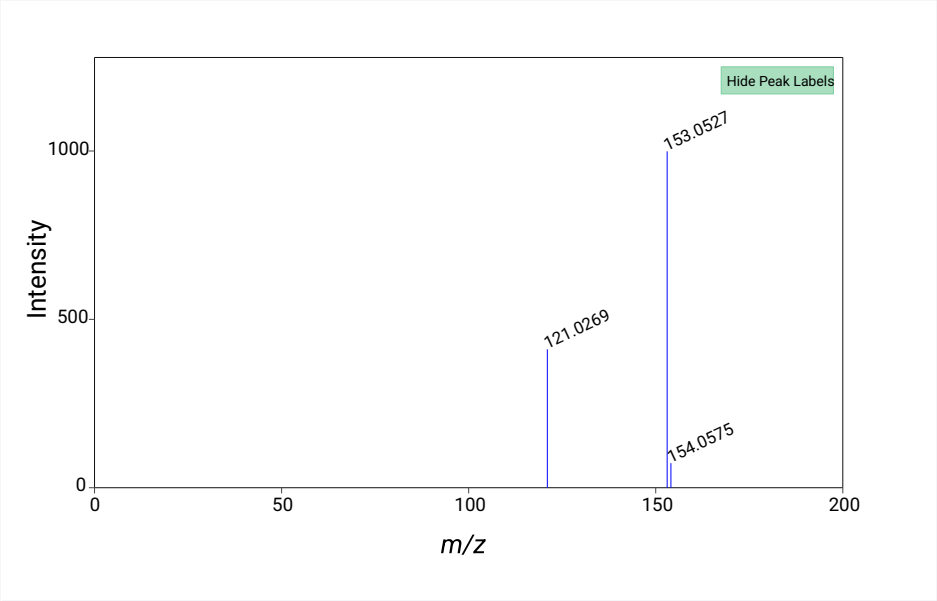


Human Metabolome Database (HMDB)

4.2.3 LC-MS

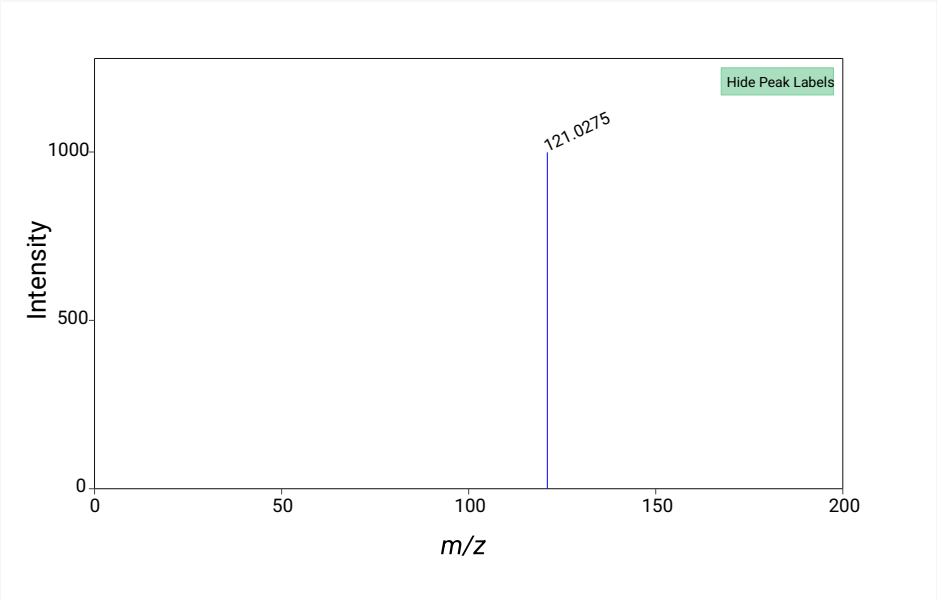
1 of 35 View All

Accession ID	MSBNK-Athens_Univ-AU237101
Authors	Nikiforos Alygizakis, Katerina Galani, Nikolaos Thomaidis, University of Athens
Instrument	Bruker maXis Impact
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	10 eV
Fragmentation Mode	CID
Column Name	Acclaim RSLC C18 2.2um, 2.1x100mm, Thermo
Retention Time	5.999 min
Precursor m/z	153.0546

Precursor Adduct	[M+H]+
Top 5 Peaks	153.0527 999 121.0269 411 154.0575 73
SPLASH	splash10-0udi-0900000000-6e5b508b9a7aa3ae3ea9
Thumbnail	
License	CC BY

▸ MassBank Europe

2 of 35	View All
Accession ID	MSBNK-Athens_Univ-AU237102
Authors	Nikiforos Alygizakis, Katerina Galani, Nikolaos Thomaidis, University of Athens
Instrument	Bruker maXis Impact
Instrument Type	LC-ESI-QTOF
MS Level	MS2
Ionization Mode	POSITIVE
Ionization	ESI
Collision Energy	20 eV
Fragmentation Mode	CID

Column Name	Acclaim RSLC C18 2.2um, 2.1x100mm, Thermo
Retention Time	6.033 min
Precursor m/z	153.0546
Precursor Adduct	[M+H]+
Top 5 Peaks	121.0275 999
SPLASH	splash10-00di-0900000000-8dd837e3f62c0c1bb90f
Thumbnail	
License	CC BY

▸ MassBank Europe

4.2.4 Other MS

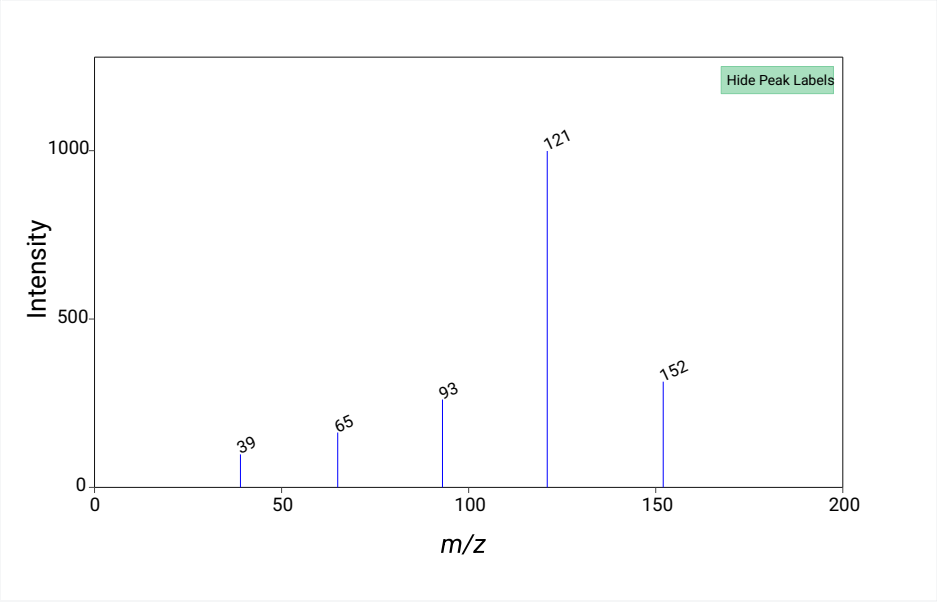
1 of 4 View All

Other MS	MASS: 68125 (NIST/EPA/MSDC Mass Spectral Database, 1990 Version); 175 (Aldermaston, Eight Peak Index of Mass)

▸ Hazardous Substances Data Bank (HSDB)

2 of 4 View All

Accession ID	MSBNK-Fac_Eng_Univ_Tokyo-JP000067

Authors	TAJIMA S, GUNMA COLLEGE OF TECHNOLOGY
Instrument	HITACHI RMU-7M
Instrument Type	EI-B
MS Level	MS
Ionization Mode	POSITIVE
Ionization	ENERGY 70 eV
Top 5 Peaks	121 999 152 314 93 261 65 163 39 98
SPLASH	splash10-00di-4900000000-5aa5692082b66b714b5d
Thumbnail	
License	CC BY-NC-SA

▸ MassBank Europe

4.3 UV Spectra

MAX ABSORPTION (ALCOHOL): 258 NM (LOG E= 4.22); SADTLER REFERENCE NUMBER: 18045 (IR, PRISM); 369 (IR, GRATING)

Weast, R.C. (ed.). Handbook of Chemistry and Physics. 60th ed. Boca Raton, Florida: CRC Press Inc.,

1979., p. C-193

▸ Hazardous Substances Data Bank (HSDB)

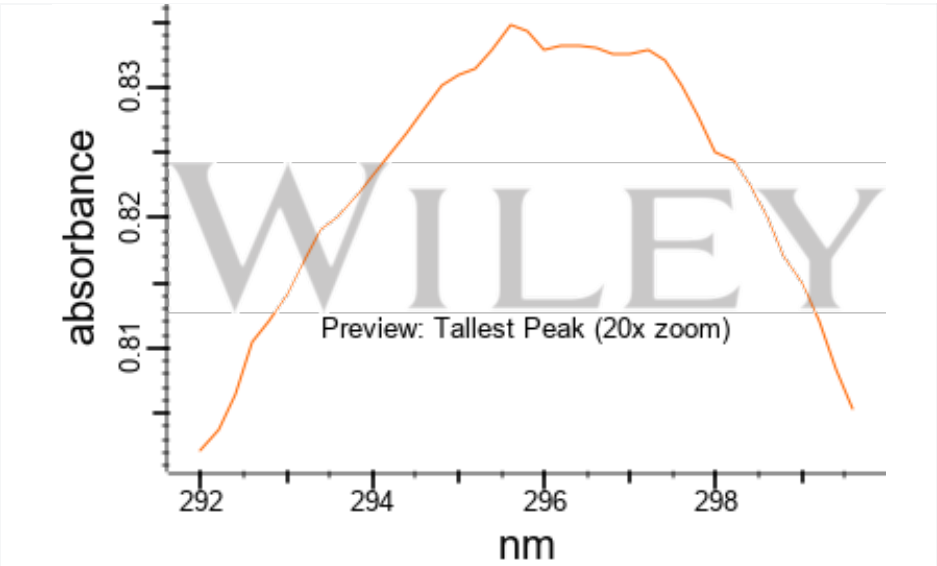
UV: 969 (Sadtler Research Laboratories Spectral Collection)

Lide, D.R., G.W.A. Milne (eds.). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V2: 1462

▸ Hazardous Substances Data Bank (HSDB)

4.3.1 UV-VIS Spectra

1 of 2

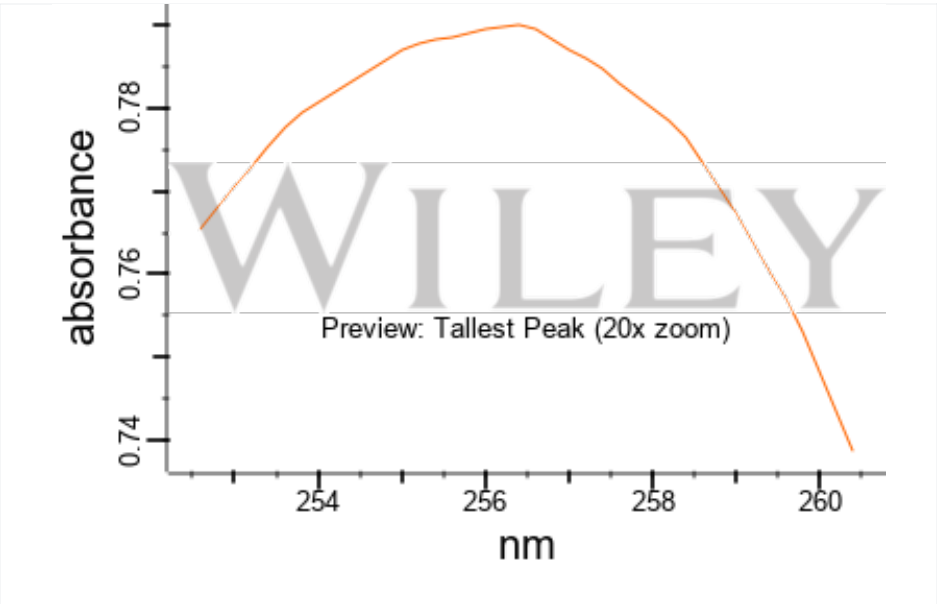
Copyright	Copyright © 2008-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

2 of 2

Copyright	Copyright © 2008-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail



▸ SpectraBase

4.4 IR Spectra

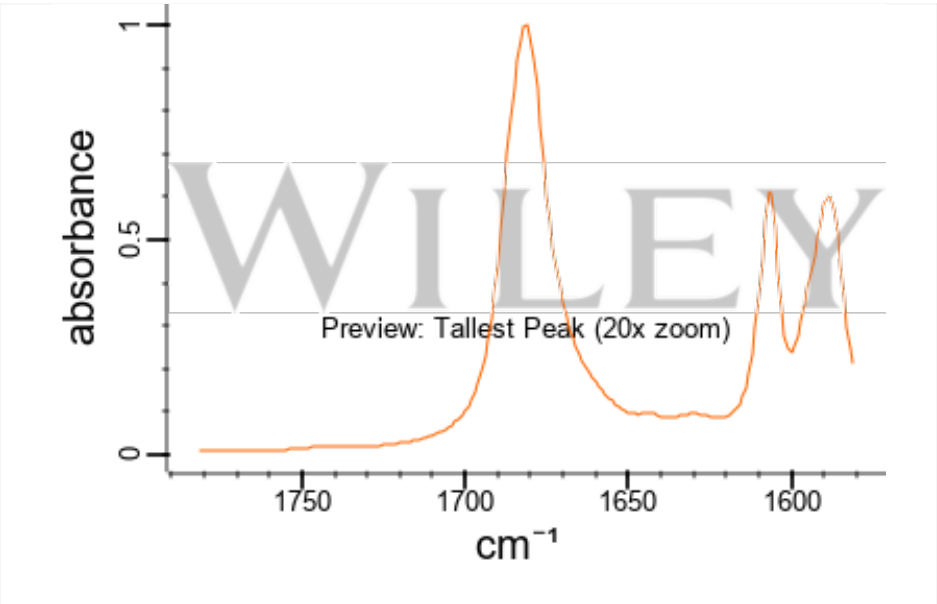
IR Spectra	IR: 6245 (Coblentz Society Spectral Collection)

▸ Hazardous Substances Data Bank (HSDB)

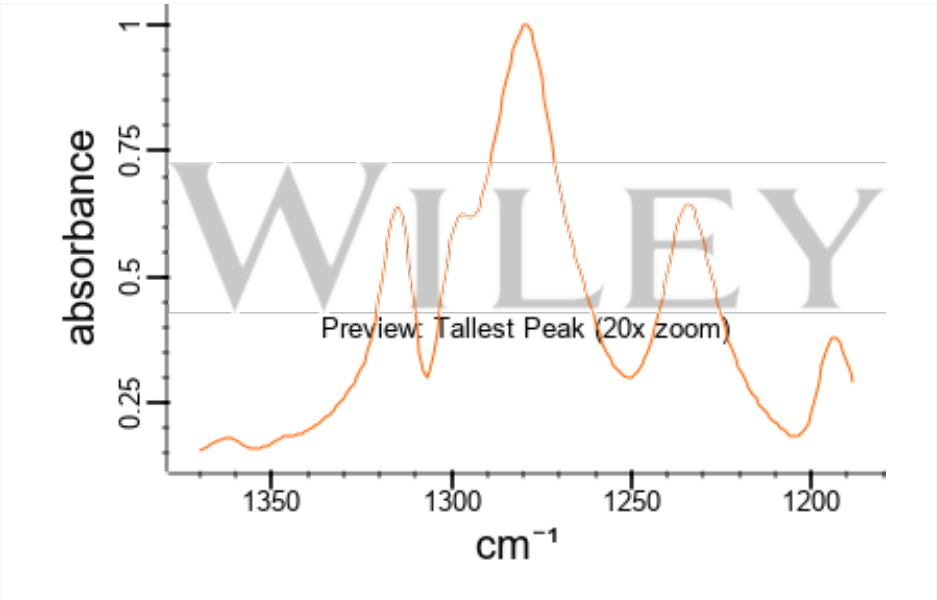
4.4.1 FTIR Spectra

1 of 2

Technique	NUJOL MULL
Source of Sample	Sprouse Scientific Systems, Inc.
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.

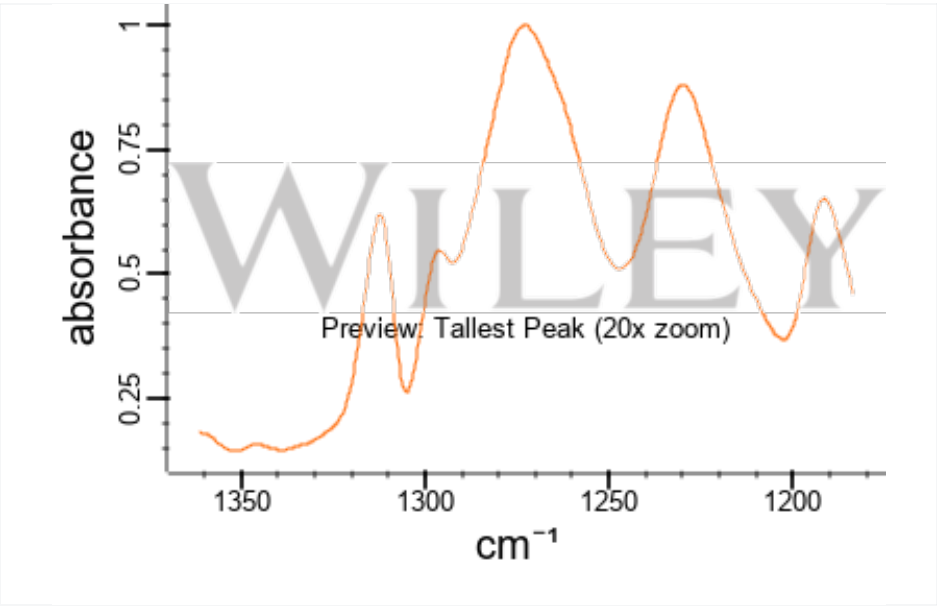
Thumbnail	

▸ SpectraBase

2 of 2	
Instrument Name	Bio-Rad FTS
Technique	KBr0
Source of Spectrum	Forensic Spectral Research
Copyright	Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

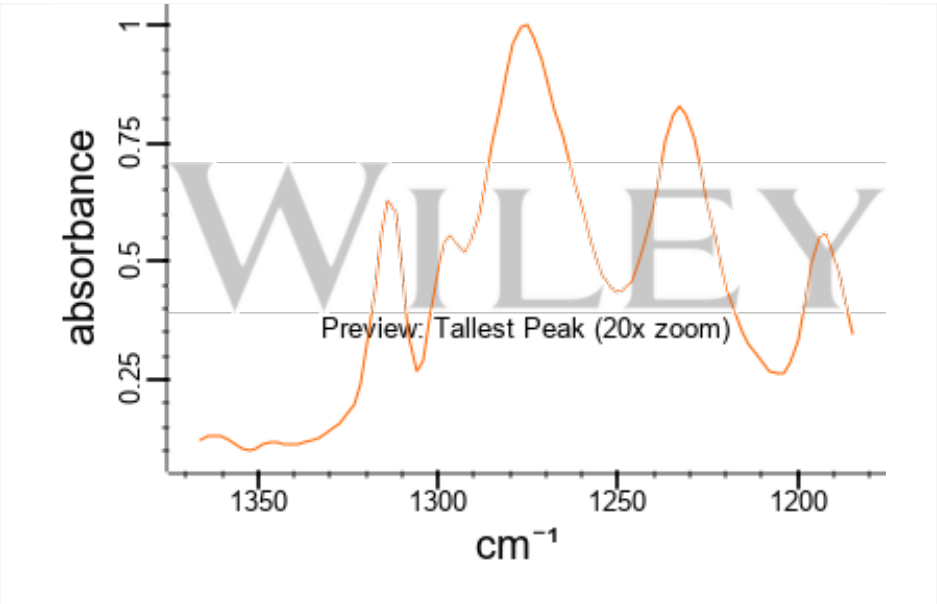
▸ SpectraBase

4.4.2 ATR-IR Spectra

1 of 2	
Instrument Name	PerkinElmer SpectrumTwo
Technique	ATR-IR
Copyright	Copyright © 2012-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

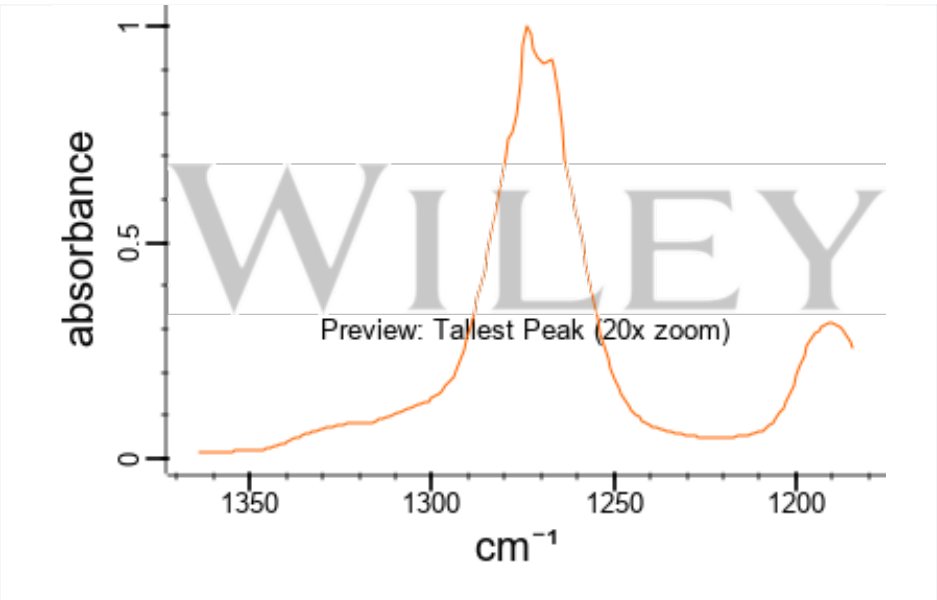
SpectraBase

2 of 2	
Instrument Name	Bio-Rad FTS
Technique	ATR-Neat (DuraSamplIR II)
Source of Spectrum	Forensic Spectral Research
Source of Sample	Spectrum Chemical Manufacturing Corp.
Catalog Number	ME163
Lot Number	UU0091
Copyright	Copyright © 2014-2024 John Wiley & Sons, Inc. All Rights Reserved.

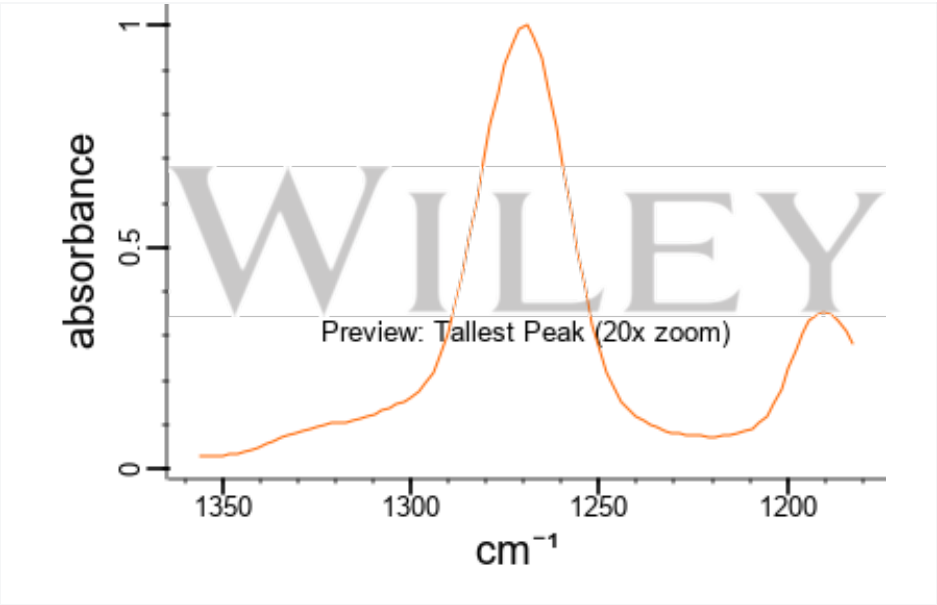
Thumbnail	

SpectraBase

4.4.3 Vapor Phase IR Spectra

1 of 2	
Instrument Name	DIGILAB FTS-14
Technique	Vapor Phase
Copyright	Copyright © 1980, 1981-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

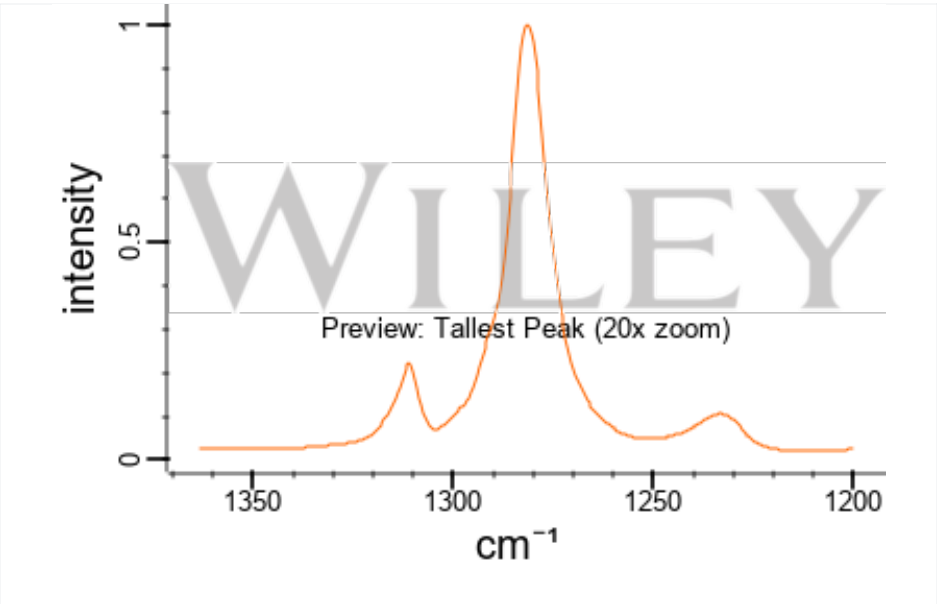
SpectraBase

2 of 2	
Source of Spectrum	Sigma-Aldrich Co. LLC.
Source of Sample	Sigma-Aldrich Co. LLC.
Catalog Number	M50109
Copyright	Copyright © 2021-2024 Sigma-Aldrich Co. LLC. - Database Compilation Copyright © 2021 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

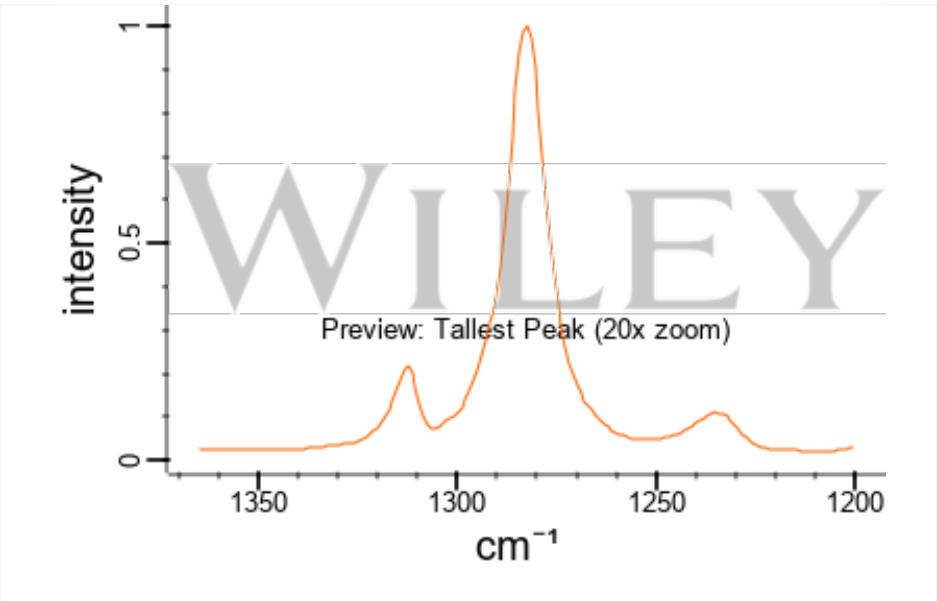
▸ SpectraBase

4.5 Raman Spectra

1 of 2	
Instrument Name	Bruker MultiRAM Stand Alone FT-Raman Spectrometer
Technique	FT-Raman
Source of Spectrum	Bio-Rad Laboratories, Inc.
Source of Sample	TCI Chemicals India Pvt. Ltd.
Catalog Number	H0216
Lot Number	GWKOH-IC
Copyright	Copyright © 2016-2024 John Wiley & Sons, Inc. All Rights Reserved.

Thumbnail	

▸ SpectraBase

2 of 2	
Technique	FT-Raman
Source of Spectrum	Forensic Spectral Research
Source of Sample	Spectrum Chemical Manufacturing Corp.
Catalog Number	ME163
Lot Number	UU0091
Copyright	Copyright © 2015-2024 John Wiley & Sons, Inc. All Rights Reserved.
Thumbnail	

▸ SpectraBase

4.6 Other Spectra

Intense mass spectral peaks: 121 m/z (100%), 152 m/z (80%), 93 m/z (70%), 65 m/z (63%)

Hites, R.A. Handbook of Mass Spectra of Environmental Contaminants. Boca Raton, FL: CRC Press Inc., 1985., p. 166

▸ Hazardous Substances Data Bank (HSDB)

5 Related Records

5.1 Related Compounds with Annotation

▸ PubChem

5.2 Related Compounds

Same Connectivity Count	9
Same Parent, Connectivity Count	56

Same Parent, Exact Count	48
Mixtures, Components, and Neutralized Forms Count	555
Similar Compounds Count	2129
Similar Conformers Count	8308

PubChem

5.3 Substances

5.3.1 PubChem Reference Collection SID

481107807

PubChem

5.3.2 Related Substances

All Count	1128
Same Count	303
Mixture Count	825

PubChem

5.3.3 Substances by Category

PubChem

5.4 Other Relationships

Butylparaben; ethylparaben; methylparaben (component of)

Alcohol; allantoin; arctium lappa root; citral; FD&C yellow NO. 5; fragrance 13576; glycerin; limonene, (+)-; methylparaben; niacinamide; panthenol; polyoxyl 40 hydrogenated castor oil; propylene glycol; riboflavin; tioxolone; water; yeast, unspecified (component of)

2,3,7,8-Tetrachlorodibenzo-P-dioxin; aluminum oxide; antipyrine; benzene; bisphenol A; carbon disulfide; carboxymethylcellulose sodium, unspecified form; diethylstilbestrol; estrone; formaldehyde; garlic; glyphosate; kerosene; methylparaben; naphthalene; paraffin; phenacetin; phenol; polytetrafluoroethylene; ptelea trifoliata bark (component of)

Arsenic trioxide; aspartame; atropa belladonna; benzalkonium chloride; chelidonium majus; formaldehyde; lycopodium clavatum spore; methylene chloride; methylparaben; phosphoric acid; phytolacca americana root; propylparaben; sodium benzoate; sodium citrate; titanium dioxide; trifolium pratense flower; zanthoxylum americanum bark; zinc oxide (component of)

PubChem

5.5 Entrez Crosslinks

PubMed Count	534
Protein Structures Count	4
Taxonomy Count	6
OMIM Count	8
Gene Count	732

▸ PubChem

6 Chemical Vendors

▸ PubChem

7 Drug and Medication Information

7.1 FDA National Drug Code Directory

- National Drug Code (NDC) Directory

7.2 Drug Labels

Drug and label

Active ingredient and drug

- DailyMed

8 Food Additives and Ingredients

8.1 Food Additive Classes

JECFA Functional Classes

Food Additives -> PRESERVATIVE;

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

8.2 FDA Substances Added to Food

Substance	METHYL P-HYDROXYBENZOATE
Used for (Technical Effect)	FLAVORING AGENT OR ADJUVANT
Document Number (21 CFR)	172.515 181.23 184.1490

- FDA Center for Food Safety and Applied Nutrition (CFSAN)

8.3 Associated Foods

FooDB

8.4 Evaluations of the Joint FAO / WHO Expert Committee on Food Additives - JECFA

Chemical Name	METHYL p-HYDROXYBENZOATE
Evaluation Year	1973
ADI	0-10 mg/kg bw
Comments	Group ADI as the sum of the ethyl and methyl esters of p-hydroxybenzoic acid. In view of the adverse effects in male rats, propyl paraben (propyl p-hydroxybenzoate) was excluded from the group ADI for the parabens used in food (TRS 940-JECFA 67/30, 2006)
Report	NMRS 53/TRS 539-JECFA 17/17
Tox Monograph	FAS 5/NMRS 53A-JECFA 17/81

Joint FAO/WHO Expert Committee on Food Additives (JECFA)

9 Agrochemical Information

9.1 Agrochemical Category

Pesticide active substances

EU Pesticides Database

9.2 EU Pesticides Data

Active Substance	methyl p-hydroxybenzoate

Status	Not approved [Reg. (EC) No 1107/2009]
Legislation	2007/442

▸ EU Pesticides Database

10 Pharmacology and Biochemistry

10.1 MeSH Pharmacological Classification

Preservatives, Pharmaceutical

Substances added to pharmaceutical preparations to protect them from chemical change or microbial action. They include ANTI-BACTERIAL AGENTS and antioxidants. (See all compounds classified as Preservatives, Pharmaceutical.)

▸ Medical Subject Headings (MeSH)

10.2 FDA Pharmacological Classification

FDA UNII	A2I8C7HI9T
Active Moiety	METHYLPARABEN
Pharmacological Classes	Established Pharmacologic Class [EPC] - Standardized Chemical Allergen
Pharmacological Classes	Physiologic Effects [PE] - Increased Histamine Release
Pharmacological Classes	Physiologic Effects [PE] - Cell-mediated Immunity
Pharmacological Classes	Chemical Structure [CS] - Allergens
FDA Pharmacology Summary	Methylparaben is a Standardized Chemical Allergen. The physiologic effect of methylparaben is by means of Increased Histamine Release, and Cell-mediated Immunity.

▸ FDA Pharm Classes

10.3 Absorption, Distribution and Excretion

By the oral route, parabens are rapidly absorbed, metabolized, and excreted. The metabolic reactions and conversions in mammals vary with the chain length of the ester, the animal species, route of administration, and quantity tested. The metabolism of parabens in humans appears to be most closely related to that of dogs. The rate of metabolite excretion appears to decrease with increasing molecular weight of the ester. /4-Hydroxybenzoates (Parabens)/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 639

▸ Hazardous Substances Data Bank (HSDB)

After methyl paraben is intravenously infused into the dog, nonhydrolyzed methyl paraben is found in brain, spleen, and pancreas. In liver, kidney, and muscle, it is immediately hydrolyzed to p-hydroxybenzoic acid ... Six hours after oral administration of 1.0 g/kg to dogs, the peak plasma concentration of free and total methyl paraben (630 and 867 ug/cu cm) is reached. After 48 hr, the vast majority was eliminated.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 664

▸ Hazardous Substances Data Bank (HSDB)

The excretion and metabolism of methylparaben were monitored in 6 preterm infants after they had received multiple doses of a gentamicin formulation containing paraben preservatives. The recovery of the paraben from urine averaged 82.6%. The urinary excretion ranged from 13.2 to 88.1%.

PMID:6631690

Hindmarsh KW et al; J Pharm Sci 72: 1039-41 (1983)

▸ Hazardous Substances Data Bank (HSDB)

... a study /was conducted/ using human volunteers in which the levels of methylparaben in the stratum corneum were measured. Cosmetic emulsions containing 0.15, 0.25, and 0.5% (w/v) methylparaben were applied one time to the forearm (42 sq cm) of one male and one female subject. At 1, 2, 5, and 12 hr after application, a small area was cleaned of emulsion using wet cotton and methylparaben was extracted by application of a glass cylinder (3.1 sq cm) with 0.5 mL ethanol for 25 min. Methylparaben concentrations were determined in the ethanol solvent using HPLC (for the 1, 2, and 5 hr durations) and GC/MS for other treatments. ... For the single application, methylparaben reached its peak 1 - 2 hr after

application (peak was slightly higher for each higher use concentration) and returned to baseline after 12 hr. /In another study,/ healthy Japanese adults (one male, eleven female) applied a lotion only (6 subjects) or a lotion and an emulsion (6 subjects) containing Methylparaben (concentration not stated) twice a day for 1 month. Concentrations of methylparaben in the stratum corneum were determined as above using GC/MS before the first application, at 1, 2, 3, and 4 weeks, and 2 days after stopping. ... Repeated applications resulted in an increase in methylparaben concentration in the stratum corneum over time for both the lotion application and the lotion plus emulsion application. After 2 days, methylparaben had returned to pretreatment levels.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 25. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

For more Absorption, Distribution and Excretion (Complete) data for METHYLPARABEN (7 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

10.4 Metabolism / Metabolites

In mice, rats, rabbits, or dogs methylparaben is excreted in the urine as unchanged benzoate, p-hydroxybenzoic acid, p-hydroxyhippuric acid (p-hydroxybenzoylglycine), ester glucuronides, ether glucuronides, or ether sulfates.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 665

▸ Hazardous Substances Data Bank (HSDB)

By the oral route, parabens are rapidly absorbed, metabolized, and excreted. The metabolic reactions and conversions in mammals vary with the chain length of the ester, the animal species, route of administration, and quantity tested. The metabolism of parabens in humans appears to be most closely related to that of dogs. The rate of metabolite excretion appears to decrease with increasing molecular weight of the ester. /4-Hydroxybenzoates (Parabens)/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 639

▸ Hazardous Substances Data Bank (HSDB)

/This study examined/ the metabolic fate of methylparaben in rabbits. The compound was given by gastric intubation, and urine was analyzed by paper chromatography. Three major metabolites, p-hydroxybenzoic acid, p-hydroxyhippuric acid, and p-carboxyphenyl glucuronide, as well as two minor metabolites, p-hydroxybenzoyl glucuronide and p-carboxyphenyl sulfate, were identified. Rabbits given orally 0.4 or 0.8 g/kg methylparaben, ethylparaben, propylparaben, or butylparaben excreted only 0.2 to 0.9% of the unchanged ester by 24 hr. Urinary excretion of p-hydroxybenzoic acid was slower with increasing carbon chain length of the paraben alkyl group. Excretion of the conjugated acid was approximately that of the free acid. At 24 hr following paraben administration, 25 to 39% was recovered as p-hydroxybenzoic acid, 15 to 29% as the glycine conjugate, 5 to 8% as the ester glucuronide, 10 to 18% as the ether glucuronide, and 7 to 12% as the sulfate.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 27. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

The metabolism of methylparaben, ethylparaben, and propylparaben was studied in rats. Animals were given orally 100 mg of ester. Blood and urine were collected regularly and analyzed by paper chromatography. Paraben metabolites were identified in the urine 30 minutes after dosing. No unchanged paraben was detected. Ninety minutes after dosing, excretion of metabolites was maximum; thereafter, excretion decreased. p-Hydroxyhippuric acid appeared in the urine after 30 minutes; its concentration then increased evenly during the next 4 hr. The glucuronide and ethereal sulfate metabolites appeared only between 30 and 75 minutes postingestion. After 90 minutes, 67 to 75% of the total paraben dose was excreted as p-hydroxybenzoic acid, 10 to 12.5% as p-hydroxyhippuric acid, and 8 to 10% as glucuronyl derivatives. The concentration of free p-hydroxybenzoic acid in the blood remained extremely low. A continuous rise occurred within the first hour, but the concentration thereafter decreased and leveled off 1 to 2 hr after ingestion. The authors concluded that there were two stages of paraben detoxification: (1) absorption of paraben and excretion in urine of p-hydroxybenzoic acid, and (2) metabolic detoxification by glucuronic-, sulfo-, and glycino-conjugation.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 27. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

For more Metabolism/Metabolites (Complete) data for METHYLPARABEN (10 total), please

visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

10.5 Mechanism of Action

...The mechanism of cytotoxic action of parabens may be linked to mitochondrial failure dependent on induction of membrane permeability transition accompanied by the mitochondrial depolarization and depletion of cellular ATP through uncoupling of oxidative phosphorylation.

PMID:12387298

Soni MG et al; Food Chem Toxicol 40 (10): 1335-73 (2002)

- Hazardous Substances Data Bank (HSDB)

10.6 Human Metabolite Information

10.6.1 Cellular Locations

Cytoplasm
Extracellular

- Human Metabolome Database (HMDB)

10.7 Biochemical Reactions

PubChem

11 Use and Manufacturing

11.1 Uses

EPA CPDat Chemical and Product Categories

The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products, Scientific Data, volume 5, Article number: 180125 (2018), DOI:10.1038/sdata.2018.125

EPA Chemical and Products Database (CPDat)

Sources/Uses

Used as a preservative in foods, cosmetics, and medicines; [HSDB] The parabens (methyl, ethyl, propyl, and butyl) were the most widely used preservatives in cosmetics (0.1% to 0.8%) until their sensitizing potential was recognized; [Marks, p. 115]

Marks - Marks JG, DeLeo VA. Contact and Occupational Dermatology, 2nd Ed. St. Louis: Mosby, 1997., p. 115

Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

For methylparaben (USEPA/OPP Pesticide Code: 061201) there are 0 labels match. /SRP: Not registered for current use in the U.S., but approved pesticide uses may change periodically and so federal, state and local authorities must be consulted for currently

approved uses./

National Pesticide Information Retrieval System's Database on Methylpaaben (99-76-3). Available from, as of October 24, 2016: https://npirspublic.ceris.purdue.edu/ppis/

▸ Hazardous Substances Data Bank (HSDB)

The active ingredient is no longer contained in any registered pesticide products ... "cancelled."

USEPA/OPP; Status of Pesticides in Registration, Reregistration and Special Review p.330 (Spring, 1998) EPA 738-R-98-002

▸ Hazardous Substances Data Bank (HSDB)

Reported uses (ppm):

Table: Reported uses (ppm): (Flavor and Extract Manufacturers' Association, 1994)

Food Category	Usual	Max.
Baked goods	0.99	0.99
Frozen dairy	0.00	0.01
Gelatins, puddings	0.00	0.01
Nonalcoholic beverages	0.00	0.01
Processed vegetables	1.00	1.00
Soft candy	0.00	0.01
Sugar substitutes	0.50	0.50

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 1297

▸ Hazardous Substances Data Bank (HSDB)

As preservative in foods, beverages and cosmetics.

O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1132

▸ Hazardous Substances Data Bank (HSDB)

For more Uses (Complete) data for METHYLPARABEN (7 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

Methylparaben is found in alcoholic beverages.

- Toxin and Toxin Target Database (T3DB)

11.1.1 Use Classification

Food additives

- EU Food Improvement Agents

Agrochemicals -> Pesticides

- EU Pesticides Database

Fragrance Ingredients

- International Fragrance Association (IFRA)

Food Additives -> PRESERVATIVE; -> JECFA Functional Classes

- Joint FAO/WHO Expert Committee on Food Additives (JECFA)

Cosmetics -> Preservative

S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) | DOI:10.5281/zenodo.2624118

- NORMAN Suspect List Exchange

11.1.2 Industry Uses

Not Known or Reasonably Ascertainable

https://www.epa.gov/chemical-data-reporting

- EPA Chemical Data Reporting (CDR)

11.1.3 Consumer Uses

Laboratory chemicals

https://www.epa.gov/chemical-data-reporting

▸ EPA Chemical Data Reporting (CDR)

11.1.4 Household Products

Household & Commercial/Institutional Products

Information on 816 consumer products that contain Methylparaben in the following categories is provided:

• Auto Products

• Commercial / Institutional

• Inside the Home

• Personal Care

• Pet Care

▸ Consumer Product Information Database (CPID)

11.2 Methods of Manufacturing

Produced by the methanol esterification of p-hydroxybenzoic acid in the presence of sulfuric acid. The materials are heated for distillation in a glass-lined reactor under reflux. The acid is then neutralized with caustic soda and the product is crystallized by cooling. The crystallized product is centrifuged, washed, dried under vacuum, milled and blended, all in corrosion-resistant equipment to avoid metallic contamination.

Burdock, G.A. (ed.). Fenaroli's Handbook of Flavor Ingredients. 6th ed.Boca Raton, FL 2010, p. 1297

▸ Hazardous Substances Data Bank (HSDB)

It is produced by the methanol esterification of p-hydroxybenzoic acid in the presence of sulfuric acid, with subsequent distillation.

21 CFR 184.1490 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 26, 2016: https://www.ecfr.gov

▸ Hazardous Substances Data Bank (HSDB)

Parabens are prepared by esterifying PHBA /parahydroxybenzoic acid/ with the corresponding alcohol in the presence of an acid catalyst, such as sulfuric acid, and an

excess of the specific alcohol. The acid is then neutralized with caustic soda, and the product is crystallized by cooling, centrifuged, washed, dried under vacuum, milled, and blended. /Parabens/

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 2. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

11.3 Formulations / Preparations

Grade: United States Pharmacopeia, FCC /Food Chemical Codex/

Larranaga, M.D., Lewis, R.J. Sr., Lewis, R.A.; Hawley's Condensed Chemical Dictionary 16th Edition. John Wiley & Sons, Inc. Hoboken, NJ 2016., p. 915

▸ Hazardous Substances Data Bank (HSDB)

Trade Names: Abiol, Aseptoform, Maseptol, Metaben, Methaben, Methyl butex, Methyl chemosept, Methyl parasept, Methylben, Metoxyde, Moldex, Nipagin, Nipagin M, Paridol, Preserval, Septos, Solbrol, Solbrol M, and Tegosept M.

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. 6:663

▸ Hazardous Substances Data Bank (HSDB)

11.4 Consumption Patterns

ESSENTIALLY 100% AS AN ANTIMICROBIAL AGENT IN FOODS & COSMETICS (1976)

SRI

▸ Hazardous Substances Data Bank (HSDB)

11.5 U.S. Production

Aggregated Product Volume

2019: <1,000,000 lb

2018: <1,000,000 lb

2017: <1,000,000 lb

2016: <1,000,000 lb

https://www.epa.gov/chemical-data-reporting

▸ EPA Chemical Data Reporting (CDR)

(1972) 4.17X10+8 GRAMS

SRI

▸ Hazardous Substances Data Bank (HSDB)

(1975) 2.21X10+8 GRAMS

SRI

▸ Hazardous Substances Data Bank (HSDB)

This chemical is listed as a High Production Volume (HPV) (65FR81686). Chemicals listed as HPV were produced in or imported into the U.S. in >1 million pounds in 1990 and/or 1994. The HPV list is based on the 1990 Inventory Update Rule. (IUR) (40 CFR part 710 subpart B; 51FR21438).

EPA/Office of Pollution Prevention and Toxics; High Production Volume (HPV) Challenge Program. Available from, as of March 14, 2007: https://www.epa.gov/hpv/pubs/general/opptsrch.htm

▸ Hazardous Substances Data Bank (HSDB)

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	>500 thousand - 1 million
1990	>1 million - 10 million
1994	>1 million - 10 million
1998	>500 thousand - 1 million
2002	10 thousand - 500 thousand

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Benzoic acid, 4-hydroxy-, methyl ester (99-76-3). Available from, as of March 6, 2007: https://www.epa.gov/oppt/iur/tools/data/2002-vol.html

▸ Hazardous Substances Data Bank (HSDB)

Non-confidential 2012 Chemical Data Reporting (CDR) information on the production and

use of chemicals manufactured or imported into the United States. Chemical: Benzoic acid, 4-hydroxy-, methyl ester. National Production Volume: Withheld.

USEPA/Pollution Prevention and Toxics; 2012 Chemical Data Reporting Database. Benzoic acid, 4-hydroxy-, methyl ester (99-76-3). Available from, as of October 26, 2016: https://java.epa.gov/oppt_chemical_search/

- Hazardous Substances Data Bank (HSDB)

11.6 General Manufacturing Information

Industry Processing Sectors

Not Known or Reasonably Ascertainable

- EPA Chemical Data Reporting (CDR)

EPA TSCA Commercial Activity Status

Benzoic acid, 4-hydroxy-, methyl ester: ACTIVE

- EPA Chemicals under the TSCA

The parabens are most active against molds and yeasts. They are less effective against bacteria, especially gram-negative bacteria. /Parabens/

Furia, T.E. (ed.). CRC Handbook of Food Additives. 2nd ed. Cleveland: The Chemical Rubber Co., 1972., p. 125

- Hazardous Substances Data Bank (HSDB)

12 Identification

12.1 Analytic Laboratory Methods

Determination of p-hydroxybenzoic acid esters in cosmetics by LC with UV and fluorescence detection /p-Hydroxybenzoic acid esters/

PMID:3417609

Akimoto N et al; J Assoc Off Anal Chem 71 (4): 823-5 (1988)

- Hazardous Substances Data Bank (HSDB)

Determination of methylparaben in liquid pharmaceutical preparations by HPLC.

Clarke G, Rashid IA; Analyst (London) 102 (1218): 685 (1977)

▸ Hazardous Substances Data Bank (HSDB)

Analyte: methylparaben; matrix: chemical identification; procedure: infrared absorption spectrophotometry with comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1160 (2007)

▸ Hazardous Substances Data Bank (HSDB)

Analyte: methylparaben; matrix: chemical purity; procedure: addition of sodium hydroxide; potentiometric titration of excess sodium hydroxide with sulfuric acid until the second point of inflection and comparison to standards

U.S. Pharmacopeia. The United States Pharmacopeia, USP 30/The National Formulary, NF 25; Rockville, MD: U.S. Pharmacopeial Convention, Inc., p1160 (2007)

▸ Hazardous Substances Data Bank (HSDB)

For more Analytic Laboratory Methods (Complete) data for METHYLPARABEN (9 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

13 Safety and Hazards

13.1 Hazards Identification

13.1.1 GHS Classification

1 of 3 View All

Pictogram(s)	Irritant
Signal	Warning
GHS Hazard Statements	H315 (78.58%): Causes skin irritation [Warning Skin corrosion/irritation] H319 (78.45%): Causes serious eye irritation [Warning Serious eye damage/ eye irritation]

	H335 (84.24%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H412 (11.18%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P261, P264, P264+P265, P271, P273, P280, P302+P352, P304+P340, P305+P351+P338, P319, P321, P332+P317, P337+P317, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)
ECHA C&L Notifications Summary	*Aggregated GHS information provided by 3277 companies from 30 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies.* *Reported as not meeting GHS hazard criteria by 1031 of 3277 companies. For more detailed information, please visit ECHA C&L website.* *Of the 29 notification(s) provided by 2246 of 3277 companies with hazard statement code(s).* *Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.*

▸ European Chemicals Agency (ECHA)

13.1.2 Hazard Classes and Categories

Skin Irrit. 2 (78.58%)

Eye Irrit. 2 (78.45%)

STOT SE 3 (84.24%)

Aquatic Chronic 3 (11.18%)

▸ European Chemicals Agency (ECHA)

Hazardous to the aquatic environment (Acute) - Category 3

Hazardous to the aquatic environment (Long-term) - Category 3

▸ NITE-CMC

13.1.3 Hazards Summary

Parabens are an uncommon cause of allergic contact dermatitis; [Marks, p. 115] Food use

limited to 0.1%; [Hawley] Observations from animal studies include mild skin and eye irritation and a low order of toxicity in high-dose oral studies; Skin sensitization has been reported from cosmetics and topical medications; A moderate eye irritant (saturated aqueous solution); Practically non-toxic in animal studies: Oral LD50 (mouse) >8000 mg/kg (Effects included flaccid paralysis and ataxia.); [HSDB] An eye and mild skin irritant; May cause skin sensitization; [eChemPortal: ERMA] Parabens can induce allergic contact dermatitis, mainly in chronic dermatitis and wounded skin. [Kanerva, p. 1822-3] An irritant; [MSDSonline]

Marks - Marks JG, DeLeo VA. Contact and Occupational Dermatology, 2nd Ed. St. Louis: Mosby, 1997., p. 115

Hawley - Lewis RJ. _Hawley's Condensed Chemical Dictionary, _15th Ed. New York: John Wiley & Sons, 2007.

Kanerva - Rustemeyer L, Elsner P, John SM, Maibach HI (eds). Kanerva's Occupational Dermatology, 2nd Ed. Berlin: Springer-Verlag, 2012., p. 1822-3

▸ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

13.1.4 Skin, Eye, and Respiratory Irritations

Methylparaben ... as saturated aq soln ... noted to be moderately irritating to eye ... .

Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 695

▸ Hazardous Substances Data Bank (HSDB)

13.2 Fire Fighting

13.2.1 Fire Fighting Procedures

Suitable extinguishing media: Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

Advice for firefighters: Wear self-contained breathing apparatus for firefighting if necessary.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8

(Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

13.3 Accidental Release Measures

13.3.1 Cleanup Methods

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided. Methods and materials for containment and cleaning up: Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

13.3.2 Disposal Methods

SRP: Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in air, soil or water; effects on animal, aquatic and plant life; and conformance with environmental and public health regulations. If it is possible or reasonable use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination.

- Hazardous Substances Data Bank (HSDB)

Product: Offer surplus and non-recyclable solutions to a licensed disposal company; Contaminated packaging: Dispose of as unused product.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

- Hazardous Substances Data Bank (HSDB)

13.3.3 Preventive Measures

ACCIDENTAL RELEASE MEASURES: Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid dust formation. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Avoid breathing dust. Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

- Hazardous Substances Data Bank (HSDB)

Precautions for safe handling: Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. Provide appropriate exhaust ventilation at places where dust is formed.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

- Hazardous Substances Data Bank (HSDB)

Appropriate engineering controls: Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

For more Preventive Measures (Complete) data for METHYLPARABEN (6 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

13.4 Handling and Storage

13.4.1 Storage Conditions

Keep container tightly closed in a dry and well-ventilated place.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

13.5 Exposure Control and Personal Protection

13.5.1 Allowable Tolerances

Residues of methyl p-hydroxybenzoate are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active)

ingredients in pesticide formulations applied to growing crops only. Use: Preservative for formulations.

40 CFR 180.920 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

▸ Hazardous Substances Data Bank (HSDB)

Residues of methyl p-hydroxybenzoate are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals. Use: Preservative. Limit: Meets specifications of Food Chemicals Codex; not to exceed 0.1% in formulations.

40 CFR 180.930 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

▸ Hazardous Substances Data Bank (HSDB)

13.5.2 Personal Protective Equipment (PPE)

Eye/face protection: Safety glasses with side-shields conforming to EN166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

Skin protection: Handle with gloves.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

Body Protection: Impervious clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

Respiratory protection: For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

13.6 Stability and Reactivity

13.6.1 Hazardous Reactivities and Incompatibilities

Incompatible materials: Strong oxidizing agents, strong bases

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

▸ Hazardous Substances Data Bank (HSDB)

13.7 Regulatory Information

REACH Registered Substance

Status: Active Update: 19-12-2022 https://echa.europa.eu/registration-dossier/-/registered-dossier/14310

Status: Active Update: 05-03-2020 https://echa.europa.eu/registration-dossier/-/registered-dossier/30649

▸ European Chemicals Agency (ECHA)

New Zealand EPA Inventory of Chemical Status

Methylparaben: Does not have an individual approval but may be used under an appropriate group standard

▸ New Zealand Environmental Protection Authority (EPA)

13.7.1 FIFRA Requirements

Residues of methyl p-hydroxybenzoate are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to growing crops only. Use: Preservative for formulations.

40 CFR 180.920 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

▸ Hazardous Substances Data Bank (HSDB)

Residues of methyl p-hydroxybenzoate are exempted from the requirement of a tolerance when used in accordance with good agricultural practice as inert (or occasionally active) ingredients in pesticide formulations applied to animals. Use: Preservative. Limit: Meets specifications of Food Chemicals Codex; not to exceed 0.1% in formulations.

40 CFR 180.930 (USEPA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

▸ Hazardous Substances Data Bank (HSDB)

As the federal pesticide law FIFRA directs, EPA is conducting a comprehensive review of older pesticides to consider their health and environmental effects and make decisions about their future use. Under this pesticide reregistration program, EPA examines health and safety data for pesticide active ingredients initially registered before November 1, 1984, and determines whether they are eligible for reregistration. In addition, all pesticides must meet the new safety standard of the Food Quality Protection Act of 1996. Pesticides for which EPA had not issued Registration Standards prior to the effective date of FIFRA, as amended in 1988, were divided into three lists based upon their potential for human exposure and other factors, with List B containing pesticides of greater concern and List D pesticides of less concern. Butyl 4-hydroxybenzoate is found on List D. Case No: 4071; Case Status: No products containing the pesticide are actively registered ... The case /is characterized/ as "cancelled." Under FIFRA, pesticide producers may voluntarily cancel their registered products. EPA also may cancel pesticide registrations if registrants fail to pay required fees or make/meet certain reregistration commitments, or if EPA reaches findings of unreasonable adverse effects.; Active ingredient (AI): Methyl 4-hydroxybenzoate; AI Status: The active ingredient is no longer contained in any registered pesticide products ... "cancelled."

USEPA/OPP; Status of Pesticides in Registration, Reregistration and Special Review p.330 (Spring, 1998) EPA 738-R-98-002

- Hazardous Substances Data Bank (HSDB)

13.7.2 FDA Requirements

Methylparaben is a food additive permitted for direct addition to food for human consumption as a synthetic flavoring substance and adjuvant in accordance with the following conditions: a) they are used in the minimum quantity required to produce their intended effect, and otherwise in accordance with all the principles of good manufacturing practice, and 2) they consist of one or more of the following, used alone or in combination with flavoring substances and adjuvants generally recognized as safe in food, prior-sanctioned for such use, or regulated by an appropriate section in this part.

21 CFR 172.515 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

- Hazardous Substances Data Bank (HSDB)

Substances classified as antimycotics, when migrating from food-packaging material shall include: methylparaben.

21 CFR 181.23 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

- Hazardous Substances Data Bank (HSDB)

Substance added directly to human food affirmed as generally recognized as safe (GRAS). The ingredient is used in food at levels not to exceed good manufacturing practices. Current good manufacturing practice results in a maximum level of 0.1 percent in food.

21 CFR 184.1490 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

- Hazardous Substances Data Bank (HSDB)

Drug products containing certain active ingredients offered over-the-counter (OTC) for certain uses. A number of active ingredients have been present in OTC drug products for various uses, as described below. However, based on evidence currently available, there are inadequate data to establish general recognition of the safety and effectiveness of these ingredients for the specified uses: methylparaben is included in topical antifungal drug products.

21 CFR 310.545(a)(22) (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

This substance is generally recognized as safe for use at a level not exceeding 0.1 percent in accordance with good manufacturing or feeding practice.

21 CFR 582.3490 (USFDA); U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from, as of October 24, 2016: https://www.ecfr.gov

Hazardous Substances Data Bank (HSDB)

13.8 Other Safety Information

13.8.1 Toxic Combustion Products

Special hazards arising from the substance or mixture: Carbon oxides

Sigma-Aldrich; Safety Data Sheet for Methyl 4-hydroxybenzoate. Product Number: H5501, Version 4.8 (Revision Date 12/18/2014). Available from, as of October 7, 2016: https://www.sigmaaldrich.com/safety-center.html

Hazardous Substances Data Bank (HSDB)

13.8.2 Special Reports

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products. Int J Toxicol 27 Suppl 4: 1-82 (2008)[Available from, as of November 21, 2016: http://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf]

Hazardous Substances Data Bank (HSDB)

14 Toxicity

14.1 Toxicological Information

14.1.1 Toxicity Summary

IDENTIFICATION AND USE: Methylparaben is a methyl ester of p-hydroxybenzoic acid. It is a stable, non-volatile compound used as an antimicrobial preservative in foods, drugs and

cosmetics. HUMAN EXPOSURE AND TOXICITY: Parabens are reported to cause contact dermatitis reactions in some individuals on cutaneous exposure. Parabens have been implicated in numerous cases of contact sensitivity associated with cutaneous exposure; however, the mechanism of this sensitivity is unknown. Sensitization has occurred when medications containing parabens have been applied to damaged or broken skin. Allergic reactions to ingested parabens have been reported, although rigorous evidence of the allergenicity of ingested paraben is lacking. ANIMAL STUDIES: Acute toxicity studies in animals indicate that methylparaben is practically non-toxic by both oral and parenteral routes. In a population with normal skin, methylparaben is practically non-irritating and non-sensitizing. In chronic administration studies, no-observed-effect levels (NOEL) as high as 1050 mg/kg have been reported and a no-observed-adverse-effect level (NOAEL) in the rat of 5700 mg/kg is posited. Methylparaben did increase chromosomal aberrations in a Chinese Hamster ovary cell assay. Methylparaben was noncarcinogenic when injected subcutaneously in mice or rats, or when administered intravaginally in rats. Methylparaben was nonteratogenic in rabbits, rats, mice, and hamsters. It is not embryotoxic. Methylparaben failed to produce any effect in uterotrophic assays in two laboratories, but did produce an effect in other studies from another laboratory. In one in vitro study, sperm were not viable at concentrations as low as 6 mg/mL methylparaben, but an in vivo study of 0.1% or 1.0% methylparaben in the diet of mice reported no spermatotoxic effects. Methylparaben was studied using rats at levels in the diet up to an estimated mean dose of 1141.1 mg/kg per day with no adverse testicular effects. ECOTOXICITY STUDIES: Medaka vitellogenin assays and DNA microarray analysis were carried out for methylparaben and found induction of significant vitellogenin in male medaka at 630 ug/L of methylparaben, while the expression levels of genes encoding proteins such as choriogenin and vitellogenin increased for concentrations at 10ug/L of methylparaben.

- Hazardous Substances Data Bank (HSDB)

14.1.2 Carcinogen Classification

Carcinogen Classification	No indication of carcinogenicity to humans (not listed by IARC).

- Toxin and Toxin Target Database (T3DB)

14.1.3 Adverse Effects

Neurotoxin - Other CNS neurotoxin

Skin Sensitizer - An agent that can induce an allergic reaction in the skin.

- Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

14.1.4 Acute Effects

6 items

Search

Compound CID	Organism	Test Type	Route	Dose	Effect	Reference
7456	rat	LD50	subcutaneous	>500 mg/kg		Clinical Toxicology., 4(2) (185), 1971
7456	mouse	LD50	oral	>8 gm/kg	PERIPHERAL NERVE AND SENSATION: FLACCID PARALYSIS WITHOUT ANESTHESIA (USUALLY NEUROMUSCULAR BLOCKAGE); BEHAVIORAL: ATAXIA	Journal of the American Pharmaceutical Association, Scientific Edition., 45(260), 1956
7456	mouse	LD50	intraperitoneal	960 mg/kg	PERIPHERAL NERVE AND SENSATION: FLACCID PARALYSIS WITHOUT ANESTHESIA (USUALLY NEUROMUSCULAR BLOCKAGE); BEHAVIORAL: SOMNOLENCE (GENERAL DEPRESSED ACTIVITY); BEHAVIORAL: ATAXIA	Journal of the American Pharmaceutical Association, Scientific Edition., 45(260), 1956

Compound CID	Organism	Test Type	Route	Dose	Effect	Reference
7456	mouse	LD50	subcutaneous	1200 mg/kg		Archives Internationales de Pharmacodynamie et de Therapie., 128(135), 1960 [PMID:13681509]
7456	rabbit	LD50	oral	6 gm/kg		FAO Nutrition Meetings Report Series., 53A(81), 1974

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▸ ChemIDplus

14.1.5 Interactions

... Using human intestinal (Caco-2) cells, it was observed that hydrolysis of parabens to p-hydroxybenzoic acid is reduced markedly by ethanol concentrations that can occur in the human intestine, 0.25-0.5% (v/v). Ethanol concentrations of 1.0-2.5% (v/v) were optimal for transesterification to ethylparaben in Caco-2 cell homogenates. The kinetics of the transesterification reaction with regard to ethanol concentration (0-20%), time, pH (3-9), protein concentration (1-5 mg/mL) and substrate concentration (6.25-200 uM) as well as the effects of different alcohols were studied. The Km and Vmax values for transesterification with ethanol for methyl, propyl, butyl, heptyl and octyl parabens were 449.7, 165.7, 86.1, 24.2 and 45.9 uM and 114.4, 37.5, 19.5, 7.5 and 7.6 umol/hr/mg Caco-2 cell protein, respectively. The Vmax values for transesterification of methylparaben with ethanol, propan-1-ol, butan-1-ol were 114.4, 5.1 and 4.9 umol/hr/mg, respectively. ... The clinical or toxicological implication is that, following co-ingestion of ester compounds with ethanol, transesterification could provide the basis for a previously unrecognized drug-alcohol interaction.

PMID:16971340

Lakeram M et al; Xenobiotica 36 (9): 739-49 (2006)

▸ Hazardous Substances Data Bank (HSDB)

... /The authors/ investigated the effects of ultraviolet-B (UVB) exposure on methylbaraben (MP)-treated human skin keratinocytes. HaCaT keratinocyte was cultured in MP-containing

medium for 24 hr, exposed to UVB (15 or 30 mJ/cm2) and further cultured for another 24 hr. Subsequent cellular viability was quantified by MTT-based assay and cell death was qualified by fluorescent microscopy and flow cytometry. ... Practical concentrations of MP (0.003%) had a little or no effect on cellular viability, oxidative stress, nitric oxide (NO) production, lipid peroxidation and activation of nuclear transcription factors in HaCaT keratinocytes. Low-dose UVB also had little or no effect on these parameters in HaCaT keratinocytes. However, UVB exposure significantly increased cell death, oxidative stress, NO production, lipid peroxidation and activation of transcription factors in MP-treated HaCaT keratinocytes. These results indicate that MP, which has been considered a safe preservative in cosmetics, may have harmful effects on human skin when exposed to sunlight.

PMID:16938376

Handa O et al; Toxicology 227 (1-2): 62-72 (2006)

▸ Hazardous Substances Data Bank (HSDB)

It has been hypothesized recently that succinylcholine-associated increases in intracranial pressure (ICP) are caused by the paraben preservatives contained in multidose vials. /The authors/ tested that hypothesis in a standard feline model to determine the effects on ICP of equal-volume injections of preservative-free succinylcholine, succinylcholine with preservatives from multi-dose vials that contain both propylparaben and methylparaben, these preservatives alone at five times the dose contained in the succinylcholine, and normal saline. The preservatives alone increased ICP by 0.08 +/- 0.08 mm Hg (+/- standard error; not significant). Normal saline had no effect on ICP. Preservative-free succinylcholine and succinylcholine with preservatives increased ICP by 4.2 +/- 0.10 and 3.8 +/- 0.07 mm Hg respectively (P less than 0.01 compared to the preservatives alone and normal saline). The 99% upper confidence limit for the increase in ICP induced by the preservatives alone was 0.42 mm Hg. This result suggests /, to the authors/ that parabens do not cause or substantially augment the ICP increase associated with succinylcholine administration.

PMID:1928776

Pompy L et al; Anesthesiology 75 (4): 669-72 (1991)

▸ Hazardous Substances Data Bank (HSDB)

To evaluate the influence of an extract of Genista tinctoria L. herba (GT) or methylparaben (MP) on histopathological changes and 2 biomarkers of oxidative stress in rats subchronicly exposed to bisphenol A (BPA). Adult female Wistar rats were orally exposed for 90 d to BPA (50 mg/kg), BPA+GT (35 mg isoflavones/kg) or BPA+MP (250 mg/kg). Plasma and tissue samples were taken from liver, kidney, thyroid, uterus, ovary, and mammary gland after 30, 60, and 90 d of exposure respectively. Lipid peroxidation and in

vivo hydroxyl radical production were evaluated by histological analysis along with malondialdehyde and 2,3-dihydroxybenzoic acid detection. The severity of histopathological changes in liver and kidneys was lower after GT treatment than after BPA or BPA+MP treatment. A minimal thyroid receptor antagonist effect was only observed after BPA+MP treatment. The abnormal folliculogenesis increased in a time-dependent manner, and the number of corpus luteum decreased. No significant histological alterations were found in the uterus. The mammary gland displayed specific estrogen stimulation changes at all periods. Both MP and GT revealed antioxidant properties reducing lipid peroxidation and BPA-induced hydroxyl radical generation. GT L. extract ameliorates the toxic effects of BPA and is proved to have antioxidant potential and antitoxic effect. MP has antioxidant properties, but has either no effect or exacerbates the BPA-induced histopathological changes.

PMID:24625398

Popa DS et al; Biomed Environ Sci 27 (2): 85-96 (2014)

▸ Hazardous Substances Data Bank (HSDB)

For more Interactions (Complete) data for METHYLPARABEN (7 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

14.1.6 Antidote and Emergency Treatment

/SRP:/ Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

▸ Hazardous Substances Data Bank (HSDB)

/SRP:/ Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if needed. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary ... . Monitor for shock and treat if

necessary ... . Anticipate seizures and treat if necessary ... . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with 0.9% saline (NS) during transport ... . Do not use emetics. For ingestion, rinse mouth and administer 5 mL/kg up to 200 mL of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool ... . Cover skin burns with dry sterile dressings after decontamination ... . /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160

▸ Hazardous Substances Data Bank (HSDB)

/SRP:/ Advanced treatment: Consider orotracheal or nasotracheal intubation for airway control in the patient who is unconscious, has severe pulmonary edema, or is in severe respiratory distress. Positive-pressure ventilation techniques with a bag valve mask device may be beneficial. Consider drug therapy for pulmonary edema ... . Consider administering a beta agonist such as albuterol for severe bronchospasm ... . Monitor cardiac rhythm and treat arrhythmias as necessary ... . Start IV administration of D5W TKO /SRP: "To keep open", minimal flow rate/. Use 0.9% saline (NS) or lactated Ringer's (LR) if signs of hypovolemia are present. For hypotension with signs of hypovolemia, administer fluid cautiously. Watch for signs of fluid overload ... . Treat seizures with diazepam or lorazepam ... . Use proparacaine hydrochloride to assist eye irrigation ... . /Poisons A and B/

Currance, P.L. Clements, B., Bronstein, A.C. (Eds).; Emergency Care For Hazardous Materials Exposure. 3rd revised edition, Elsevier Mosby, St. Louis, MO 2007, p. 160-1

▸ Hazardous Substances Data Bank (HSDB)

14.1.7 Human Toxicity Excerpts

/HUMAN EXPOSURE STUDIES/ In vitro studies suggest that the preservatives methylparaben and propylparaben included in some multidose vials of succinylcholine are the cerebral vasodilators responsible for the increases in intracranial pressure (ICP) documented after succinylcholine administration. To test this hypothesis, ... cerebral blood flow (CBF) and cerebral blood flow velocity (CBFV) with inhaled 133-Xenon and transcranial Doppler /were measured/ respectively in healthy humans before and after the intravenous administration of methylparaben and propylparaben. ... No change /was found/ in either CBF or CBFV after the paraben injections and therefore /it was/ concluded that it is unlikely that the rise in ICP seen with succinylcholine is caused by cerebral arterial vasodilatation from the preservatives methylparaben and propylparaben.

PMID:1394758

Gelb AW et al; Can J Anaesth 39 (7): 691-4 (1992)

▸ Hazardous Substances Data Bank (HSDB)

/HUMAN EXPOSURE STUDIES/ ... Methylparaben, ethylparaben, propylparaben, and butylparaben were each applied to the backs of 50 humans at concentrations of 5, 7, 10, 12, and 15 percent in propylene glycol. Test compounds were applied daily for 5 days, and patches were then removed and the sites scored. The concentrations of individual parabens that produced no irritation were methylparaben, 5 %; ethylparaben, 7 %; propylparaben, 12 5% and butylparaben, 5%. Higher concentrations produced some evidence of irritation. In a repeated insult patch test (RIPT), each paraben at the "no effect" concentration above was applied to the skin of 50 subjects (25M/25F) for 4 to 8 hr every other day for 3 weeks (10 applications). Following a 3-week rest, the materials were reapplied at induction concentrations for 24 to 48 hr. No sensitization was reported.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 56. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

/HUMAN EXPOSURE STUDIES/ Methylparaben and ethylparaben, in increasing concentrations, were studied for their effect on the oral mucous membrane of 39 subjects. They described toxic limit concentrations for methylparaben and ethylparaben of 5 and 10%, respectively. One subject had a reaction of the oral mucous membrane to methylparaben.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 57. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

/SIGNS AND SYMPTOMS/ ... used in region of eyes ... occasionally cause redness & swelling of eyelids from allergic contact dermatitis.

Grant, W.M. Toxicology of the Eye. 3rd ed. Springfield, IL: Charles C. Thomas Publisher, 1986., p. 695

▸ Hazardous Substances Data Bank (HSDB)

For more Human Toxicity Excerpts (Complete) data for METHYLPARABEN (27 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

14.1.8 Non-Human Toxicity Excerpts

/LABORATORY ANIMALS: Acute Exposure/ The ciliotoxicity of methyl-p-hydroxybenzoate and propyl hydroxybenzoate was investigated /via inhalation exposures to male Wistar rats/. It is shown that at the concentrations used (0.28 and 0.38 mM) propyl hydroxybenzoate exerted only mild toxicity. The methy-p-hydroxybenzoate solutions used (1.18 and 2.36 mM) were much more ciliotoxic. There was, however, an order of magnitude difference in the concentrations used as a result of constraints imposed by their differing aqueous solubilities. There was no evidence of synergism in the ciliotoxicity of the two compounds when the methyl-p-hydroxybenzoate concentration was raised from 1.18 to 2.36 mM and the propyl hydroxybenzoate concentration was raised from 0.28 to 0.38 mM in a 2(2) factorial experiment. At those levels the two compounds showed additive effects. On the other hand, clear synergism was evidenced by the fact that the ciliotoxicity of both methyl-p-hydroxybenzoate and propyl hydroxybenzoate was dependent on whether the cilia were exposed to each hydroxybenzoate singly or in combination.

PMID:8095540

Jian L, Po LW; J Pharm Pharmacol 45 (2): 98-101 (1993)

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ At LD50 either oral or ip admin in mice, methylparaben causes flaccid paralysis. /From table/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 665

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ Methylparaben in 0.85% saline was administered orally to groups of 5 to 10 rats at doses of 100 to 5000 mg/kg. Animals were observed for 10 days and then killed. All 10 animals receiving 5000 mg/kg died within 24 hours. Necropsy findings included reddened gastric mucosa and congested lungs. No animals died at 100 and 500 mg/kg.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 34. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

/LABORATORY ANIMALS: Acute Exposure/ Methylparaben as a 21.8% saline suspension / was administered/ orally to each of 10 rats at a dose of 5000 mg/kg. Animals were

observed for 7 days and then killed. No toxicity, abnormal behavior, or gross lesions were observed. Methylparaben at 37 to 79% was administered orally to groups of six male rats at doses of 2600 to 5600 mg/kg. Animals were observed for 7 days and then killed. No toxicity, abnormal behavior, or gross lesions were observed. The authors concluded that the rat acute oral LD for 21.8 to 79% methylparaben was > 5600 mg/kg.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 34. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Excerpts (Complete) data for METHYLPARABEN (34 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

14.1.9 Non-Human Toxicity Values

LD50 Rat oral >5600 mg/kg for 21.8 to 79% methylparaben in saline.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 34. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

LD50 Rat oral 2100 mg/kg for methylparaben as a 0.85% saline suspension.

Cosmetic Ingredient Review; Final Amended Report on the Safety Assessment of Methylparaben, Ethylparaben, Propylparaben, Isopropylparaben, Butylparaben, Isobutylparaben, and Benzylparaben as used in Cosmetic Products p 34. Int J Toxicol 27 Suppl 4: 1-82 (2008). Available from, as of November 21, 2016: https://online.personalcarecouncil.org/ctfa-static/online/lists/cir-pdfs/PR427.pdf

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mouse oral 8.0 g/kg /From table/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 665

▸ Hazardous Substances Data Bank (HSDB)

LD50 Mouse ip 0.96 g/kg /From table/

Bingham, E.; Cohrssen, B.; Powell, C.H.; Patty's Toxicology Volumes 1-9 5th ed. John Wiley & Sons. New York, N.Y. (2001)., p. V6 665

▸ Hazardous Substances Data Bank (HSDB)

For more Non-Human Toxicity Values (Complete) data for METHYLPARABEN (9 total), please visit the HSDB record page.

▸ Hazardous Substances Data Bank (HSDB)

14.1.10 Ecotoxicity Values

EC50; Species: Daphnia magna (Water Flea); Conditions: freshwater, static, pH 7.6-8.0, dissolved oxygen 100% saturated; Concentration: 11400 ug/L for 24 hr (95% confidence interval: 10600-47600 ug/L); Effect: intoxication, immobilization /formulation/

Madsen T et al; Ministry of the Environment and Energy, Danish EPA, Environmental Project No.615: 235 (2001) as cited in the ECOTOX database. Available from, as of October 6, 2016

▸ Hazardous Substances Data Bank (HSDB)

EC50; Species: Daphnia magna (Water Flea); Conditions: freshwater, static, pH 7.6-8.0, dissolved oxygen 100% saturated; Concentration: 11200 ug/L for 24 hr (95% confidence interval: 5730-22000 ug/L); Effect: intoxication, immobilization /formulation/

Madsen T et al; Ministry of the Environment and Energy, Danish EPA, Environmental Project No.615: 235 (2001) as cited in the ECOTOX database. Available from, as of October 6, 2016

▸ Hazardous Substances Data Bank (HSDB)

EC50; Species: Daphnia magna (Water Flea)age <24 hr neonate; Conditions: freshwater, static, 21 °C, pH 7.45, hardness 100 mg/L CaCO3; Concentration: 70000 ug/L for 24 hr; Effect: intoxication, immobilization /99% purity/

Kamaya Y et al; Chemosphere 59 (2): 255-61 (2005) as cited in the ECOTOX database. Available from, as of October 6, 2016

▸ Hazardous Substances Data Bank (HSDB)

EC50; Species: Daphnia magna (Water Flea)age <24 hr neonate; Conditions: freshwater, static, 21 °C, pH 7.45, hardness 100 mg/L CaCO3; Concentration: 41100 ug/L for 48 hr; Effect: intoxication, immobilization /99% purity/

Kamaya Y et al; Chemosphere 59 (2): 255-61 (2005) as cited in the ECOTOX database. Available from, as of October 6, 2016

- Hazardous Substances Data Bank (HSDB)

For more Ecotoxicity Values (Complete) data for METHYLPARABEN (7 total), please visit the HSDB record page.

- Hazardous Substances Data Bank (HSDB)

14.1.11 Ecotoxicity Excerpts

/AQUATIC SPECIES/ The acute toxicity of 21 parabens and their chlorinated derivatives was investigated by means of two toxicity bioassays: Daphnia magna immobilization test and the inhibition of bioluminescence of Vibrio fischeri. The median effective concentration (EC(50)) values of the tested parabens ranged from 2.2 to 62 mg/L in the D. magna test and from 0.0038 to 5.9 mg/L in the V. fischeri test at 15 min after exposure. The toxicity of dichlorinated methyl- and n-propylparaben, the most commonly used preservatives in cosmetics, toward D. magna was 3.9- and 2.8-fold that of their corresponding parent compounds. Toxicity toward D. magna showed a linear relationship with log P, indicating that toxicity increases with increasing hydrophobicity. On the other hand, the correlations of toxicity toward V. fischeri with hydrophobicity and with the degree of chlorination were poor. In addition, the results of the present study indicated that the V. fischeri test was more sensitive than the D. magna test for the determination of the acute toxicity of parabens. A complete assessment of the ecological and toxicological risks of parabens may require the examination of chlorinated parabens as well as the parent pollutants, as described in the present study.

PMID:19089854

Terasaki M et al; J Appl Toxicol 29 (3): 242-7 (2009)

- Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ The chronic toxicity of 12 compounds of parabens and their chlorinated by-products was investigated using 7-day Ceriodaphnia dubia test under static renewal condition in order to generate information on how to disinfect by-products of preservatives that are discharged in aquatic systems. The mortality and inhibition of reproduction tended to increase with increasing hydrophobicity and decreased with the degree of chlorination of parabens. The EC50 values for mortality, offspring number, and first brood production ranged between 0.30-3.1, 0.047-12, and 1.3-6.3 mg/L, respectively. For the number of neonates, the most sensitive endpoint, the no-observed-effect concentration (NOEC) and lowest-observed-effect concentration (LOEC) values ranged from 0.63 to 10 mg/L and from 1.2 to 19 mg/L, respectively. Methylparaben (MP),

benzylparaben (BnP), and dichlorinated BnP (Cl2BnP) elicited a significant decrease in offspring numbers even at their lowest concentration tested; the NOEC for these compounds was determined to be less than the lowest test concentration (1.3, 0.04, and 0.63 mg/L for MP, BnP, and Cl2BnP, respectively). Propylparaben (PP), chlorinated PP, isopropylparaben (iPP), and chlorinated iPP exhibited nonmonotonic concentration-dependent response; their NOEC and LOEC values could not be determined. The multivariate approach involving principal component analysis and hierarchical cluster analysis revealed four groups that corresponded to the toxicological profiles of parabens. Our results suggested that disinfection of parabens by chlorination could reduce aquatic toxicity of original compounds. The findings obtained in our study together with the data available on paraben concentrations in aquatic systems can be used to perform preliminary risk assessment by comparing the predicted environmental concentration (PEC) with the predicted no-effect concentration (PNEC) for the marine aquatic environment. The calculated PEC/PNEC ratios ranged from 0.0012 to 0.2, with the highest value observed in MP. This suggested that there are negligible environmental risks for aquatic organisms at current use levels.

Terasaki M et al; Environ Toxicol 30 (6): 664-73 (2015)

▸ Hazardous Substances Data Bank (HSDB)

/AQUATIC SPECIES/ In the present study, aquatic concentrations of seven parabens were determined in urban streams highly affected by treated or untreated domestic sewage in Tokushima and Osaka, Japan. The detected highest concentrations were 670, 207, and 163ng/L for methylparaben, n-propylparaben, and n-butylparaben, respectively in sampling sites with watershed area of no sewer system in Tokushima. Conventional acute/chronic toxicity tests were conducted using medaka (Oryzias latipes), Daphnia magna, and Psuedokirchneriella subcapitata for four parabens, which was consistent with our previous study on three parabens, n-butylparaben, i-butylparaben, and benzylparaben. The aquatic toxicity on fish, daphnia, and algae was weaker for the parabens with a shorter alkyl chain than those with a longer alkyl chain as predicted by their hydrophobicity. Medaka vitellogenin assays and DNA microarray analysis were carried out for methylparaben and found induction of significant vitellogenin in male medaka at 630ug/L of methylparaben, while the expression levels of genes encoding proteins such as choriogenin and vitellogenin increased for concentrations at 10ug/L of methylparaben. Measured environmental concentrations (MECs) of seven parabens in Tokushima and Osaka were divided by predicted no effect concentrations (PNECs) and hazard quotient (MEC/PNEC) was determined for individual parabens. The MEC/PNEC was highest for n-propylparaben and was 0.010 followed by n-butylparaben (max. of 0.0086) and methylparaben (max. of 0.0042). The sum of the MEC/PNEC for the seven parabens was 0.0049. Equivalence factors were assigned for each paraben on the basis of the toxicity of n-butylparabenfor

each species, and n-butylparaben equivalence was calculated for the measured environmental concentrations. The MEC/PNEC approach was also conducted for the n-butylparaben-based equivalence values. The maximum MEC/PNEC was 0.018, which is lower than the trigger level for further detailed study such as large-scale monitoring for chronic toxicity tests including full-life cycle tests for fish.

PMID:22051549

Yamamoto H et al; Sci Total Environ 410-411: 102-11 (2011)

▸ Hazardous Substances Data Bank (HSDB)

14.1.12 Ongoing Test Status

EPA has released the Interactive Chemical Safety for Sustainability (iCSS) Dashboard. The iCSS Dashboard provides an interactive tool to explore rapid, automated (or in vitro high-throughput) chemical screening data generated by the Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration. /The title compound was tested by ToxCast and/or Tox21 assays/[USEPA; ICSS Dashboard Application; Available from, as of September 8, 2016: http://actor.epa.gov/dashboard/]

▸ Hazardous Substances Data Bank (HSDB)

14.2 Ecological Information

14.2.1 Environmental Fate / Exposure Summary

Methylparaben's production and use as a yeast and mold inhibitor, a transporting agent for ophthalmic solutions, preservative for foods, beverages, and cosmetics and a preservative in topical pharmaceuticals may result in its release to the environment through various waste streams. If released to air, an estimated vapor pressure of 2.4X10-4 mm Hg at 25 °C indicates methylparaben will exist in both the vapor and particulate phases in the atmosphere. Vapor-phase methylparaben will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be one day. Particulate-phase methylparaben will be removed from the atmosphere by wet and dry deposition. Methylparaben contains chromophores that absorb at wavelengths >290 nm and, therefore, may be susceptible to direct photolysis by sunlight. If released to soil, methylparaben is expected to have high mobility based upon an estimated Koc of 87. The pKa of methylparaben is 8.5, indicating that this compound will exist partially in the anion form in the environment and anions generally do not adsorb

more strongly to soils containing organic carbon and clay than their neutral counterparts. Volatilization from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 2.3X10-9 atm-cu m/mole. Methylparaben is not expected to volatilize from dry soil surfaces based upon its vapor pressure. Using the Zahn-Wellens test, 100% biodegradation was observed in 6 days following a 2-day acclimation period suggesting that biodegradation may be an important environmental fate process in soil and water. If released into water, methylparaben is not expected to adsorb to suspended solids and sediment based upon the estimated Koc. Volatilization from water surfaces is not expected to be an important fate process based upon this compound's estimated Henry's Law constant. An estimated BCF of 9 suggests the potential for bioconcentration in aquatic organisms is low. Although hydrolysis of methylparaben is possible at elevated temperatures, it is not expected to be an important fate process under environmental conditions. Occupational exposure to methylparaben may occur through inhalation and dermal contact with this compound at workplaces where methylparaben is produced or used. Monitoring and use data indicate that the general population may be exposed via dermal contact with products containing this compound, ingestion of some foods, inhalation of and contact with house dust and administration of pharmaceutical products. (SRC)

▸ Hazardous Substances Data Bank (HSDB)

14.2.2 Artificial Pollution Sources

Methylparaben's production and use as a yeast and mold inhibitor(1), a transporting agent for ophthalmic solutions(2), preservative for foods, beverages, and cosmetics(3), and a preservative in parenteral solutions, topical antibiotic or corticosteroid preparations, galencials(4) may result in its release to the environment through various waste streams(SRC).

(1) Ellenhorn MJ et al; Medical Toxicology. New York, NY: Elsevier Science Publishing Co, Inc; p. 1206 (1988) (2) McEvoy GK, ed; American Hospital Formulary Service; AHFS Drug Information. American Society of Health-System Pharmacists, Bethesda, MD; p. 412 (2006) (3) O'Neil MJ, ed; The Merck Index. 15th ed., Cambridge, UK: Royal Society of Chemistry, p. 1132 (2013) (4) David RM et al; Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th ed. (1999-2016). New York, NY: John Wiley & Sons, Inc. On-line Posting Date: 17 Aug 2012

▸ Hazardous Substances Data Bank (HSDB)

14.2.3 Environmental Fate

TERRESTRIAL FATE: Based on a classification scheme(1), an estimated Koc value of

87(SRC), determined from a structure estimation method(2), indicates that methylparaben is expected to have high mobility in soil(SRC). The estimated pKa of methylparaben is 8.5(3), indicating that this compound will exist partially in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4). Volatilization of methylparaben from moist soil surfaces is not expected to be an important fate process(SRC) given an estimated Henry's Law constant of 2.2X10-9 atm-cu m/mole(SRC), using a fragment constant estimation method(5). Methylparaben is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2.4X10-4 mm Hg at 25 °C(SRC), determined from a fragment constant method(2). Using the Zahn-Wellens test, 100% biodegradation was observed in 6 days following a 2-day acclimation period(6) suggesting that biodegradation may be an important environmental fate process in soil(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (3) ACE; ACE and JChem acidity and basicity calculator. ACE UKY-4.0. 2005-2015. Marvin JS. ChemAxon. Available from, as of Nov 2, 2016: https://epoch.uky.edu/ace/public/pKa.jsp (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000) (5) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (6) Wellens H; Z Wasser Abwasser Forch 23: 85-98 (1990)

▸ Hazardous Substances Data Bank (HSDB)

AQUATIC FATE: Based on a classification scheme(1), an estimated Koc value of 87(SRC), determined from a structure estimation method(2), indicates that methylparaben is not expected to adsorb to suspended solids and sediment(SRC). Volatilization from water surfaces is not expected(3) based upon an estimated Henry's Law constant of 2.2X10-9 atm-cu m/mole(SRC), developed using a fragment constant estimation method(4). According to a classification scheme(5), an estimated BCF of 9(SRC), from its log Kow of 1.96(6) and a regression-derived equation(2), suggests the potential for bioconcentration in aquatic organisms is low(SRC). Using the Zahn-Wellens test, 100% biodegradation was observed in 6 days following a 2-day acclimation period(7) suggesting that biodegradation may be an important environmental fate process in water(SRC).

(1) Swann RL et al; Res Rev 85: 17-28 (1983) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (4) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (5) Franke C et al; Chemosphere 29: 1501-14 (1994) (6) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 42 (1995) (7) Wellens H; Z Wasser Abwasser Forch 23: 85-98 (1990)

▸ Hazardous Substances Data Bank (HSDB)

ATMOSPHERIC FATE: According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere(1), methylparaben, which has an estimated vapor pressure of 2.4X10-4 mm Hg at 25 °C(SRC), determined from a fragment constant method(2), will exist in both the vapor and particulate phases in the ambient atmosphere. Vapor-phase methylparaben is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals(SRC); the half-life for this reaction in air is estimated to be one day(SRC), calculated from its rate constant of 1.1X10-11 cu cm/ molecule-sec at 25 °C(SRC) that was derived using a structure estimation method(3). Particulate-phase methylparaben may be removed from the air by wet and dry deposition(SRC). Methylparaben contains chromophores that absorb at wavelengths >290 nm(4) and, therefore, may be susceptible to direct photolysis by sunlight(SRC).

(1) Bidleman TF; Environ Sci Technol 22: 361-367 (1988) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (3) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

▸ Hazardous Substances Data Bank (HSDB)

14.2.4 Environmental Biodegradation

AEROBIC: Methylparaben degraded 100% after 6 days with a 2 day acclimation period in sludge inoculum using the Zahn-Wellens test(1) which requires a 0.2 - 1.0 g/L dry inolculum and 50-400 dissolved organic carbon/L test concentration(2). Based on this data methylparaben is expected to biodegrade readily in the environment(SRC). Average concentrations of not detected, 2.8, 1.61 and 2.5 ng/L were reported for methylparaben in gray water from 32 residences and associated effluent from aerobic, anaerobic and anaerobic+aerobic biological treatment systems, respectively. Testing was done in August, 2008 in Sneek, The Netherlands(3). Methylparaben, present at an average concentration of 4200 ng/L, exhibited half-lives of 1.8 days and 35.2 hours using an activated sludge batch test and a real wastewater treatment plant test, respectively; sampling was conducted during April and May 2010 in a metropolitan area of northwest Spain(4).

(1) Wellens H; Z Wasser Abwasser Forch; 23: 85-98 (1990) (2) Boethling RS, Mackay D; Handbook of Property Estimation Methods for Chemicals. Boca Raton, FL: Lewis Pub p. 291 (2000) (3) Hernandez Leal L et al; Environ Sci Technol 44(17): 6835-6842 (2010) (4) Gonzalez-Marino I et al; Water Res 45(20): 6770-6780 (2011)

▸ Hazardous Substances Data Bank (HSDB)

14.2.5 Environmental Abiotic Degradation

The rate constant for the vapor-phase reaction of methylparaben with photochemically-produced hydroxyl radicals has been estimated as 1.1X10-11 cu cm/molecule-sec at 25 °C(SRC) using a structure estimation method(1). This corresponds to an atmospheric half-life of about one day at an atmospheric concentration of 5X10+5 hydroxyl radicals per cu cm(1). A base-catalyzed second-order hydrolysis rate constant of 6.4X10-3 L/mole-sec(SRC) was estimated using a structure estimation method(2); this corresponds to half-lives of 36 and 3.5 years at pH values of 7 and 8, respectively(2). At an elevated temperature of 130.5 °C, hydrolysis half-lives of 22.5 hrs, 4.47 hrs, and 45.3 min were observed in phosphate buffered solutions with pH levels of 5.89, 6.58, and 7.75, respectively(3). Hydrolysis half-lives of 31.4 min, 25.0 min, 20.8 min, 19.7 min, 10.9 min at pH levels of 7.67, 7.93, 8.06, 8.19, and 8.76, respectively, were also observed at the same temperature(3). Although hydrolysis of methylparaben is possible, it is not expected to be an important fate process under environmental conditions(SRC). Methylparaben contains chromophores that absorb at wavelengths >290 nm and therefore may be susceptible to direct photolysis by sunlight(4).

(1) Meylan WM, Howard PH; Chemosphere 26: 2293-99 (1993) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (3) Sunderland VB et al; Int J Pharm 19: 1-15 (1984) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 8-12 (1990)

▸ Hazardous Substances Data Bank (HSDB)

14.2.6 Environmental Bioconcentration

An estimated BCF of 9 was calculated in fish for methylparaben(SRC), using a log Kow of 1.96(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

(1) Hansch C et al; Exploring QSAR. Hydrophobic, Electronic, and Steric Constants. ACS Prof Ref Book. Heller SR, consult. ed., Washington, DC: Amer Chem Soc p. 42 (1995) (2) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (3) Franke C et al; Chemosphere 29: 1501-14 (1994)

▸ Hazardous Substances Data Bank (HSDB)

14.2.7 Soil Adsorption / Mobility

Using a structure estimation method based on molecular connectivity indices(1), the Koc of methylparaben can be estimated to be 87(SRC). According to a classification scheme(2), this estimated Koc value suggests that methylparaben is expected to have high mobility in

soil. The estimated pKa of methylparaben is 8.5(3), indicating that this compound will exist partially in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(4).

(1) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) ACE; ACE and JChem acidity and basicity calculator. ACE UKY-4.0. 2005-2015. Marvin JS. ChemAxon. Available from, as of Nov 2, 2016: https://epoch.uky.edu/ace/public/pKa.jsp (4) Doucette WJ; pp. 141-188 in Handbook of Property Estimation Methods for Chemicals. Boethling RS, Mackay D, eds. Boca Raton, FL: Lewis Publ (2000)

▸ Hazardous Substances Data Bank (HSDB)

14.2.8 Volatilization from Water / Soil

The Henry's Law constant for methylparaben is estimated as 2.2X10-9 atm-cu m/mole(SRC) using a fragment constant estimation method(1). This Henry's Law constant indicates that methylparaben is expected to be essentially nonvolatile from water and moist soil surfaces(2). Methylparaben is not expected to volatilize from dry soil surfaces(SRC) based upon an estimated vapor pressure of 2.4X10-4 mm Hg(SRC), determined from a fragment constant method(3).

(1) Meylan WM, Howard PH; Environ Toxicol Chem 10: 1283-93 (1991) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Washington, DC: Amer Chem Soc pp. 15-1 to 15-29 (1990) (3) US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.1. Nov, 2012. Available from, as of Nov 2, 2016: https://www2.epa.gov/tsca-screening-tools

▸ Hazardous Substances Data Bank (HSDB)

14.2.9 Environmental Water Concentrations

GROUNDWATER: Methylparaben was present in 44 of 448 samples of groundwater sampled in the UK from 1992 to 2009. The maximum concentration reported was 5 ug/L(1).

(1) Stuart M et al; Sci Total Environ 416: 1-21 (2012)

▸ Hazardous Substances Data Bank (HSDB)

DRINKING WATER: The average concentration of methylparaben from 8 drinking water samples from different cities in the Turia River Basin, Spain was 12 ng/L (6 samples positive). The average concentration in mineral waters was 40 ng/L (11 of 11 samples positive). Sampling was conducted in October, 2012; limit of quantitation = 0.2(1).

(1) Carmona E et al; Sci Total Environ 484: 53-63 (2014)

- Hazardous Substances Data Bank (HSDB)

SURFACE WATER: Methylbaraben was detected in the Turia River, Valencia, Spain. The average concentration from 22 samples was 119 ng/L (17 samples positive). Sampling was conducted in October, 2012; limit of quantitation = 2.0(1).

(1) Carmona E et al; Sci Total Environ 484: 53-63 (2014)

- Hazardous Substances Data Bank (HSDB)

14.2.10 Effluent Concentrations

The average concentration of methylparaben in 21 influent and effluent samples from wastewater treatment plants on the Turia River, Valencia, Spain were 334 ng/L (21 samples positive) and 11 ng/L (21 samples positive), respectively. Sampling was conducted in October, 2012; limit of quantitation effluent = 1.0(1). The compound was detected at a range of 2642-11,601, <3-50 and <0.3-68 ng/L in influent, final effluent and surface waters, respectively, in the UK(2).

(1) Carmona E et al; Sci Total Environ 484: 53-63 (2014) (2) Petrie B et al; Water Res 72: 3-27 (2015)

- Hazardous Substances Data Bank (HSDB)

14.2.11 Sediment / Soil Concentrations

SEDIMENT: The average concentration of methylparaben from 22 sediment samples from the Turia River, Valencia, Spain was 152 ng/g (17 samples positive). Sampling was conducted in October, 2012; limit of quantitation = 2.4(1).

(1) Carmona E et al; Sci Total Environ 484: 53-63 (2014)

- Hazardous Substances Data Bank (HSDB)

14.2.12 Other Environmental Concentrations

Methylparaben concentrations in 158 indoor dust samples (13 cities, 4 countries) from the United States, China, Korea and Japan(1).

Country	No Samples	Median concn (ng/g)	Range (ng/g)	Detection Rate (%)
USA	40	760	39-14,300	100

Country	No Samples	Median concn (ng/g)	Range (ng/g)	Detection Rate (%)
China	55	320	20-7170	100
Korea	41	1310	240-7200	100
Japan	22	1470	209-11,300	100

(1) Wang L et al; Environ Sci Technol 46: 11584-93 (2012)

▸ Hazardous Substances Data Bank (HSDB)

14.2.13 Probable Routes of Human Exposure

NIOSH (NOES Survey 1981-1983) has statistically estimated that 590,361 workers (398,916 of these are female) are potentially exposed to methylparaben in the US(1). Occupational exposure to methylparaben may occur through dermal contact with this compound at workplaces where methylparaben is produced or used(SRC). Monitoring and use data indicate that the general population may be exposed via dermal contact with products containing this compound, ingestion of some foods, inhalation of and contact with house dust and administration of pharmaceutical products(SRC).

(1) NIOSH; NOES. National Occupational Exposure Survey conducted from 1981-1983. Estimated numbers of employees potentially exposed to specific agents by 2-digit standard industrial classification (SIC). Available from, as of Jan 9, 2007: https://www.cdc.gov/noes/

▸ Hazardous Substances Data Bank (HSDB)

14.2.14 Average Daily Intake

Estimated daily intakes of methylparaben from indoor dust (13 cities, 4 countries) from the United States, China, Korea and Japan (all ng/kg bw/day)(1).

Population	USA	China	Korea	Japan
Infants	2.35	Not reported	Not reported	Not reported
Toddlers	2.80	Not reported	Not reported	Not reported
Children	1.40	0.53	3.24	3.90
Teenagers	0.55	Not reported	Not reported	Not reported
Adults	0.22	0.11	0.66	0.86

(1) Wang L et al; Environ Sci Technol 46: 11584-93 (2012)

▸ Hazardous Substances Data Bank (HSDB)

14.2.15 Body Burden

Methylparaben had a frequency of detection of 99% in urine samples from a group of US male and female adults sampled from 2003 to 2005(1).

(1) Ye X et al; Environ Health Perspect 114(12): 1843-46 (2006)

▸ Hazardous Substances Data Bank (HSDB)

Concentration of urinary p-hydroxybenzoic acid and methylparaben in children and adults from the United States and China(1).

Sample population	Concn Urinary Parabens & p-hydroxybenzoic acid (umol/L)	Methylparaben daily intake (mg/day)
US girls	6.69	0.66
US boys	6.22	0.56
Chinese girls	13.2	0.50
Chinese boys	11.3	0.66
Chinese adult females	27.9	5.12
Chinese adult males	10.4	1.59

(1) Wang L et al; Environ Sci Technol 47: 2069-76 (2013)

▸ Hazardous Substances Data Bank (HSDB)

15 Associated Disorders and Diseases

14 items

Search

Disease	Evidence Type	Evidence PMID
Abnormalities, Multiple	marker/mechanism	23637088

Disease	Evidence Type	Evidence PMID
		29360218
Attention Deficit Disorder with Hyperactivity	marker/mechanism	32283359
Birth Weight	marker/mechanism	25061923 32283359
Cognition Disorders	therapeutic	23068419
Dermatitis, Allergic Contact	marker/mechanism	26795242

First Previous Page 1 of 3 Next Last

▸ Comparative Toxicogenomics Database (CTD)

Associated Occupational Diseases with Exposure to the Compound

Contact dermatitis, allergic [Category: Skin Disease]

▸ Haz-Map, Information on Hazardous Chemicals and Occupational Diseases

Disease	References
Colorectal cancer	PubMed: 7482520, 22148915, 19006102, 23940645, 24424155, 20156336, 19678709, 25105552, 21773981, 25037050, 27015276, 27107423, 27275383, 28587349 Silke Matysik, Caroline Ivanne Le Roy, Gerhard Liebisch, Sandrine Paule Claus. Metabolomics of fecal samples: A practical consideration. Trends in Food Science & Technology. Vol. 57, Part B, Nov. 2016, p.244-255: http://www.sciencedirect.com/science/article/pii/S0924224416301984
Cystic fibrosis	PubMed: 7119120, 15185309, 20347721 Adriana Nori de Macedo. Robust capillary electrophoresis methods for biomarker discovery and routine measurements in clinical and epidemiological applications. March 2017: https://macsphere.mcmaster.ca/handle/11375/21248

▸ Human Metabolome Database (HMDB)

16 Literature

16.1 Consolidated References

3,949 items

Search SORT BY Publication Date - Most Recent

A stability indicating RP-HPLC-UV assay method for the simultaneous determination of hydroquinone, tretinoin, hydrocortisone, butylated hydroxytoluene and parabens in pharmaceutical creams

Publication Date: 2024-05-15

PMID: 38354540 **DOI:** 10.1016/j.jpba.2024.116021

Determination of parabens in breast milk using stir bar sorptive extraction coupled with UHPLC-UV

Publication Date: 2024-04-01

PMID: 38159355 **DOI:** 10.1016/j.talanta.2023.125609

Occurrence profiling, risk assessment, and correlations of antimicrobials in surface water and groundwater systems in Southwest Nigeria

Publication Date: 2024-03-20

PMID: 38323594 **DOI:** 10.1039/d3em00516j

Association of serum bisphenols, parabens, and triclosan concentrations with Sjögren Syndrome in the Hangzhou, China population

Publication Date: 2024-03-10

PMID: 38220002 **DOI:** 10.1016/j.scitotenv.2024.170031

An integrated transcriptome-microbiome host relationship associated with paraben toxicity in the brackish water flea Diaphanosoma celebensis

Publication Date: 2024-03-05

PMID: 38232552 **DOI:** 10.1016/j.jhazmat.2024.133512

First Previous Page 1 of 790 Next Last

PubChem

16.2 NLM Curated PubMed Citations

All NLM Curated PubMed Citations

PubChem

16.3 Springer Nature References

3,025 items

Search SORT BY Publication Date - Oldest

Efficient Removal of Methylparaben from an Aqueous Stream Using Waste Tamarind Fruit Shell as a Biosorbent
Publication Date: 2023
Publication Name: Water, Air, & Soil Pollution

Methylparaben induces cell-cycle arrest and caspase-3-mediated apoptosis in human placental BeWo cells
Publication Date: 2020
Publication Name: Molecular & Cellular Toxicology

Association between urinary methylparaben level and bone mineral density in children and adolescents aged 8–19 years
PMID: 37749468
Publication Date: 2023
Publication Name: Environmental Science and Pollution Research

Development and validation of a new method for determination of methylparaben in Iran market infant formulae by HPLC
Publication Date: 2021
Publication Name: Journal of Environmental Health Science and Engineering

The correlation between ROS generation and LPO process as the function of methylparaben concentrations during hemoglobin fructation
Publication Date: 2020
Publication Name: Journal of the Iranian Chemical Society

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Springer Nature

16.4 Thieme References

42 items

Search SORT BY Publication Date - Most Recent

A Mild Heteroatom (O-, N-, and S-) Methylation Protocol Using Trimethyl Phosphate (TMP)–

Ca(OH)2Combination
DOI: 10.1055/a-1731-3852
Publication Date: 2022
Publication Name: Synthesis

Helical Carbenium Ion-Based Organic Photoredox Catalyst: A Versatile and Sustainable Option in Red-Light-Induced Reactions
DOI: 10.1055/s-0040-1705942
Publication Date: 2021
Publication Name: Synlett

Substitution of Arylboronic Acids
Publication Date: 2018
Publication Name: Science of Synthesis

Photocatalysis
Publication Date: 2018
Publication Name: Science of Synthesis

A Negotiation between Different Nucleophiles in SNAr Reactions
DOI: 10.1055/s-0036-1589929
Publication Date: 2017
Publication Name: Synfacts

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Thieme Chemistry

16.5 Wiley References

- Wiley

16.6 Chemical Co-Occurrences in Literature

- PubChem

16.7 Chemical-Gene Co-Occurrences in Literature

PubChem

16.8 Chemical-Disease Co-Occurrences in Literature

PubChem

17 Patents

17.1 Depositor-Supplied Patent Identifiers

- PubChem

Link to all deposited patent identifiers

- PubChem

17.2 WIPO PATENTSCOPE

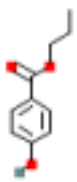
Patents are available for this chemical structure:

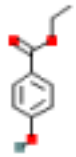
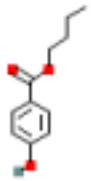
https://patentscope.wipo.int/search/en/result.jsf?inchikey=LXCFILQKKLGQFO-UHFFFAOYSA-N

- PATENTSCOPE (WIPO)

17.3 Chemical Co-Occurrences in Patents

Showing 3 of 100 View More

Chemical	Selected evidence
	4,321 patents from 3,554 patent families View Top 1000 Sustained-release buprenorphine formulations US-10744132-B2; Grant Date: 2020-08-18 Method of ultrasonic coupling

Chemical	Selected evidence
Propylparaben CID 7175	US-3710779-A; Grant Date: 1973-01-16 Defoaming device for medical humidifier US-3793810-A; Grant Date: 1974-02-26
 Ethylparaben CID 8434	1,181 patents from 961 patent families View Top 1000 Method for prevention or treatment of degenerative neurologial brain disorders US-9040580-B2; Grant Date: 2015-05-26 Topical formulation of 3-(2,2,2-trimethylhydrazinium) propionate dihydrate EP-2340016-B1; Grant Date: 2013-01-23 Antibacterial resin composition and molded article JP-3981997-B2; Grant Date: 2007-09-26
 Butylparaben CID 7184	1,057 patents from 894 patent families View Top 1000 Skin protective gel containing polyvinyl methylether or monoisopropyl ester of polyvinyl methylether maleic acid US-3876771-A; Grant Date: 1975-04-08 Scorch inhibitors for bisphenol-cured fluoroelastomers US-6486247-B1; Grant Date: 2002-11-26 Long-acting colloidal insulin formulation and its preparation US-8017156-B2; Grant Date: 2011-09-13

▸ PubChem

17.4 Chemical-Disease Co-Occurrences in Patents

Showing 3 of 100 View More

Disease	Selected evidence
Skin Diseases	1,102 patents from 951 patent families View Top 1000 Brimonidine gel compositions and methods of use US-10201517-B2; Grant Date: 2019-02-12

Disease	Selected evidence
	Gel compositions and methods of use US-8163725-B1; Grant Date: 2012-04-24 Disinfectant for the surface of human body parts containing hydrogen peroxide US-3954974-A; Grant Date: 1976-05-04
Acne Vulgaris	690 patents from 558 patent families View All Soy depigmenting and skin care compositions EP-1139974-B2; Grant Date: 2018-11-28 How to Treat Acne Vulgaris Using Topical Dapsone Compositions JP-6951332-B2; Grant Date: 2021-10-20 Delivery of active ingredients from plant materials to skin US-10052269-B2; Grant Date: 2018-08-21
Dermatitis	713 patents from 599 patent families View All Topical solubilized ivermectin for inflammatory skin conditions US-11235061-B1; Grant Date: 2022-02-01 Composition for elimination of fine dust and adding of moisture to skin using antioxidant saponin KR-102122757-B1; Grant Date: 2020-06-17 Healing composition employing an enzyme-modified casein US-5166132-A; Grant Date: 1992-11-24

▸ PubChem

17.5 Chemical-Gene Co-Occurrences in Patents

Showing 3 of 100 View More

Gene	Selected evidence
elastin	330 patents from 289 patent families View All Mask pack using temperature-responsive sol-gel transfer hydro-

Gene	Selected evidence
	gel KR-101502912-B1; Grant Date: 2015-03-16 Temperature Sensitive State-Changing Hydrogel Composition and Method for their Preparation KR-100506543-B1; Grant Date: 2005-08-05 A cosmetic mask filled with structured gel KR-102332347-B1; Grant Date: 2021-11-30
insulin	496 patents from 374 patent families View All Methods of delivering stable topical drug compositions US-9060925-B2; Grant Date: 2015-06-23 Long-acting colloidal insulin formulation and its preparation US-8017156-B2; Grant Date: 2011-09-13 Stable topical drug delivery composition JP-5241995-B2; Grant Date: 2013-07-17
ervk-25	533 patents from 366 patent families View All Soy depigmenting and skin care compositions EP-1139974-B2; Grant Date: 2018-11-28 Enzymatic detergent US-8420584-B2; Grant Date: 2013-04-16 Enzymatic detergent US-7211552-B1; Grant Date: 2007-05-01

▸ PubChem

18 Interactions and Pathways

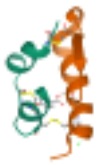
18.1 Protein Bound 3D Structures

4 items

E. coli GyrB ATPase domain in complex with methyl 4-hydroxybenzoate

PDB Code: 7DQU

Resolution: 1.88 Å



X-RAY CRYSTALLOGRAPHIC STUDIES ON HEXAMERIC INSULINS IN THE PRESENCE OF HELIX-STABILIZING AGENTS, THIOCYANATE, METHYLPARABEN AND PHENOL

PDB Code: 3MTH

Resolution: 1.9 Å

Crystal structure of P.aeruginosa LpxC in complex with inhibitor

PDB Code: 7CIA

Resolution: 1.92 Å

Crystal structure form ultalente insulin microcrystals

PDB Code: 2VK0

Resolution: 2.2 Å

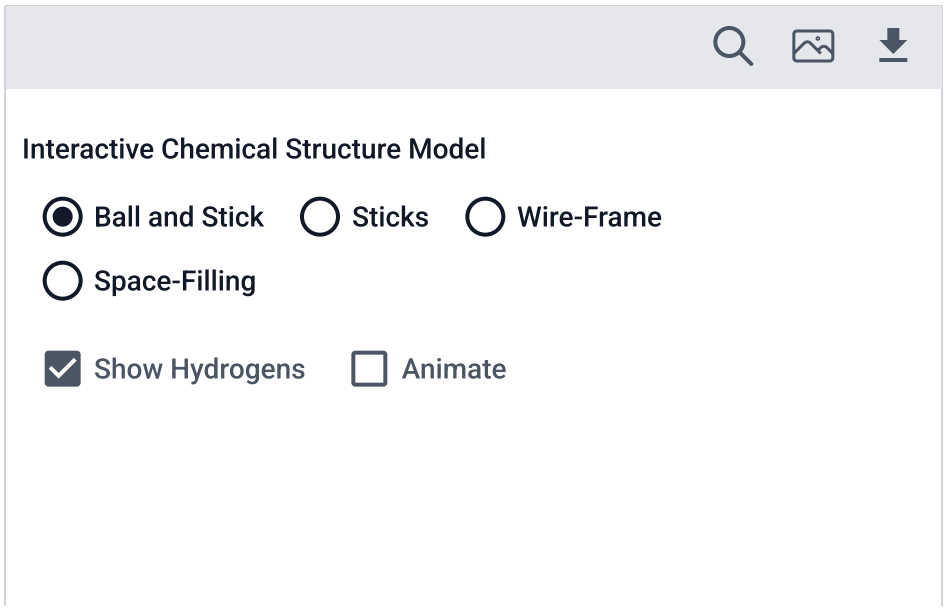
▸ RCSB Protein Data Bank (RCSB PDB)

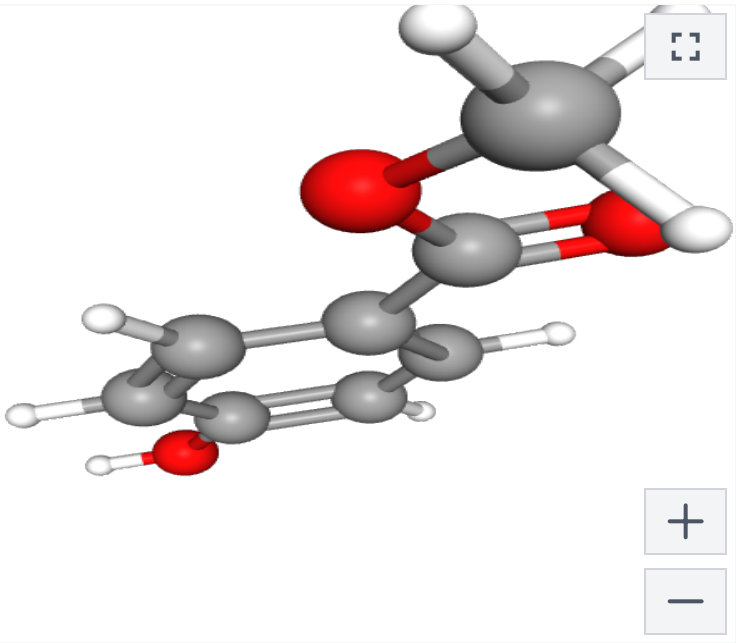
View 4 proteins in NCBI Structure

▸ PubChem

18.1.1 Ligands from Protein Bound 3D Structures

PDBe Ligand Code	MPB
PDBe Structure Code	3MTH
PDBe Conformer	



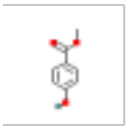
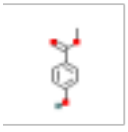


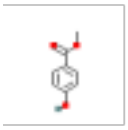
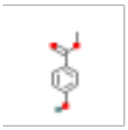
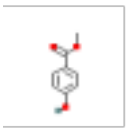
▸ Protein Data Bank in Europe (PDBe)

18.2 Chemical-Target Interactions

755 items

Search SORT BY Data Source - A to Z

Structure	Protein	Gene	Taxonomy	Action	Evidence IDs	Data Source
	Transient receptor potential cation channel subfamily A member 1	TRPA1	Homo sapiens (human)	Activator		Therapeutic Target Database (TTD)
	Transient receptor potential cation channel subfamily A member 1	Trpa1	Mus musculus (house mouse)	Activation	PMID:17351650	IUPHAR/BPS Guide to PHARMACOLOGY

Structure	Protein	Gene	Taxonomy	Action	Evidence IDs	Data Source
		NFE2L2	Homo sapiens (human)			Drug Gene Interaction database (DGIdb)
	Carbonic anhydrase 1	CA1	Homo sapiens (human)		PMID:22668600	Toxin and Toxin Target Database (T3DB)
	Carbonic anhydrase 12	CA12	Homo sapiens (human)		PMID:22668600	Toxin and Toxin Target Database (T3DB)

First Previous Page 1 of 151 Next Last

Comparative Toxicogenomics Database (CTD); Drug Gene Interaction database (DGIdb); IUPHA...

18.3 Pathways

PubChem

19 Biological Test Results

19.1 BioAssay Results

PubChem

20 Taxonomy

- KNApSAcK Species-Metabolite Database; LOTUS - the natural products occurrence database; N...

21 Classification

21.1 MeSH Tree

- Medical Subject Headings (MeSH)

21.2 NCI Thesaurus Tree

NCI Thesaurus (NCIt)

21.3 ChEBI Ontology

ChEBI

21.4 KEGG: JP15

KEGG

21.5 FDA Pharm Classes

FDA Pharm Classes

21.6 ChemIDplus

ChemIDplus

21.7 IUPHAR / BPS Guide to PHARMACOLOGY Target

Classification

IUPHAR/BPS Guide to PHARMACOLOGY

21.8 ChEMBL Target Tree

ChEMBL

21.9 UN GHS Classification

GHS Classification (UNECE)

21.10 EPA CPDat Classification

EPA Chemical and Products Database (CPDat)

21.11 NORMAN Suspect List Exchange Classification

- NORMAN Suspect List Exchange

21.12 EPA DSSTox Classification

- EPA DSSTox

21.13 Consumer Product Information Database Classification

- Consumer Product Information Database (CPID)

21.14 LOTUS Tree

- LOTUS - the natural products occurrence database

21.15 EPA Substance Registry Services Tree

EPA Substance Registry Services

22 Information Sources

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https://pubchem.ncbi.nlm.nih.gov/substance/?source=chemidplus&sourceid=0000099763

ChemIDplus Chemical Information Classification
https://pubchem.ncbi.nlm.nih.gov/source/ChemIDplus

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https://dtp.cancer.gov/dtpstandard/servlet/dwindex?searchtype=NSC&outputformat=html&searchlist=3827

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https://comptox.epa.gov/dashboard/DTXSID4022529

CompTox Chemicals Dashboard Chemical Lists

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https://echa.europa.eu/substance-information/-/substanceinfo/100.002.532

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https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/40334

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https://www.fda.gov/about-fda/about-website/website-policies#linking

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https://gsrs.ncats.nih.gov/ginas/app/beta/substances/A2I8C7HI9T

10. Hazardous Substances Data Bank (HSDB)

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https://pubchem.ncbi.nlm.nih.gov/source/hsdb/1184

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https://www.epa.govt.nz/industry-areas/hazardous-substances/guidance-for-importers-and-manufacturers/

hazardous-substances-databases/

14. ChEBI

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https://www.ebi.ac.uk/chebi/searchId.do?chebiId=CHEBI:31835

ChEBI Ontology

http://www.ebi.ac.uk/chebi/userManualForward.do#ChEBI%20Ontology

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https://dailymed.nlm.nih.gov/dailymed/browse-drug-classes.cfm

FDA Pharmacological Classification

https://www.fda.gov/ForIndustry/DataStandards/StructuredProductLabeling/ucm162549.htm

16. LOTUS - the natural products occurrence database

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https://lotus.nprod.net/

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https://www.wikidata.org/wiki/Q229987

LOTUS Tree

https://lotus.naturalproducts.net/

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http://www.t3db.ca/toxins/T3D3977

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https://www.ebi.ac.uk/chembl/compound_report_card/CHEMBL325372/

ChEMBL Protein Target Tree

https://www.ebi.ac.uk/chembl/g/#browse/targets

19. Comparative Toxicogenomics Database (CTD)

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20. Drug Gene Interaction database (DGIdb)

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http://www.dgidb.org/downloads

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https://www.dgidb.org/drugs/rxcui:29903

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https://www.guidetopharmacology.org/GRAC/LigandDisplayForward?ligandId=6273

Guide to Pharmacology Target Classification

https://www.guidetopharmacology.org/targets.jsp

22. Therapeutic Target Database (TTD)

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https://idrblab.net/ttd/data/drug/details/D0T3NP

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https://haz-map.com/Agents/6133

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https://www.whatsinproducts.com/contents/view/1/6

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https://www.whatsinproducts.com/chemicals/view/1/773/000099-76-3

Consumer Products Category Classification

https://www.whatsinproducts.com/

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https://www.crystallography.net/cod/4507504.html

https://www.crystallography.net/cod/4507505.html

https://www.crystallography.net/cod/4507506.html

26. The Cambridge Structural Database

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=617627

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=696528

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=905982

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=905983

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=905984

https://www.ccdc.cam.ac.uk/structures/Search?Ccdcid=822737

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https://dailymed.nlm.nih.gov/dailymed/search.cfm?labeltype=all&query=METHYLPARABEN

28. EPA Chemical and Products Database (CPDat)

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https://comptox.epa.gov/dashboard/DTXSID4022529#exposure

EPA CPDat Classification

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

29. EU Food Improvement Agents

METHYL p-HYDROXYBENZOATE

https://eur-lex.europa.eu/legal-content/EN/ALL/?uri=CELEX%3A32012R0231

30. EU Pesticides Database

Methyl p-hydroxybenzoate

https://ec.europa.eu/food/plant/pesticides/eu-pesticides-database/active-substances/?event=as.details&as_id=223

31. Joint FAO/WHO Expert Committee on Food Additives (JECFA)

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https://www.norman-network.com/nds/SLE/

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https://www.nite.go.jp/chem/english/ghs/08-meti-0050e.html

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METHYL P-HYDROXYBENZOATE

https://www.cfsanappsexternal.fda.gov/scripts/fdcc/index.cfm?set=FoodSubstances&id=METHYLHYDROXYBENZOATE

35. Flavor and Extract Manufacturers Association (FEMA)

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https://www.femaflavor.org/flavor-library/methyl-p-hydroxybenzoate

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https://foodb.ca/compounds/FDB010509

37. NMRShiftDB

https://pubchem.ncbi.nlm.nih.gov/substance/588052

38. MassBank Europe

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https://github.com/MassBank/MassBank-web/blob/main/MassBank-Project/LICENSE.txt

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https://massbank.eu/MassBank/Result.jsp?inchikey=LXCFILQKKLGQFO-UHFFFAOYSA-N

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https://mona.fiehnlab.ucdavis.edu/spectra/browse?query=exists(compound.metaData.name:%27InChIKey%27%20and%20compound.metaData.value:%27LXCFILQKKLGQFO-UHFFFAOYSA-N%27)

40. NIST Mass Spectrometry Data Center

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https://www.nist.gov/srd/public-law

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http://www.nist.gov/srd/nist1a.cfm

41. SpectraBase

4-HYDROXYBENZOIC ACID, METHYL ESTER
https://spectrabase.com/spectrum/8rp7YOCXr3a

METHYL 4-HYDROXYBENZOATE
https://spectrabase.com/spectrum/KLFSTTVZ4zj

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/GCPTWX64Hf6

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/42Kkz9SxtDC

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/Htbud7nUd5c

BENZOIC ACID, 4-HYDROXY-, METHYL ESTER
https://spectrabase.com/spectrum/2hAdauLK1ai

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/Jd6h0Bur5Tx

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/3fBd7HV6rpp

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/7uPMOSA0URf

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/9lFysySERRu

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/IEnx6Rps2vF

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/CtM6Jb8OjhB

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/C4uYD3PcNru

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/LumSubJ6Vbe

Methyl 4-hydroxybenzoate
https://spectrabase.com/spectrum/HI5UIoT43qx

Methylparaben
https://spectrabase.com/spectrum/6CGYHayETXx

42. ## Japan Chemical Substance Dictionary (Nikkaji)

http://jglobal.jst.go.jp/en/redirect?Nikkaji_No=J3.996I

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https://www.kegg.jp/entry/D01400

Drugs listed in the Japanese Pharmacopoeia
http://www.genome.jp/kegg-bin/get_htext?br08311.keg

44. ## KNApSAcK Species-Metabolite Database

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http://www.knapsackfamily.com/knapsack_core/info.php?sname=C_ID&word=C00030751

45. ## Natural Product Activity and Species Source (NPASS)

Methylparaben
https://bidd.group/NPASS/compound.php?compoundID=NPC131192

46. ## Kruve Lab, Ionization & Mass Spectrometry, Stockholm University

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47. ## Metabolomics Workbench

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https://www.metabolomicsworkbench.org/data/StructureData.php?RegNo=45617

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https://rxnav.nlm.nih.gov/id/rxnorm/29903

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https://pharos.nih.gov/ligands/AYT63ZDRP3G6

52. Protein Data Bank in Europe (PDBe)

http://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/MPB

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https://www.rcsb.org/pages/policies

https://www.rcsb.org/

54. Springer Nature

https://pubchem.ncbi.nlm.nih.gov/substance/?source=15745&sourceid=11042984-410172207

55. SpringerMaterials

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https://materials.springer.com/substanceprofile/docs/smsid_gmqhuueqqmcnqydy

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58. Wikipedia

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59. Wiley

https://pubchem.ncbi.nlm.nih.gov/substance/?source=wiley&sourceid=155073

60. PubChem

https://pubchem.ncbi.nlm.nih.gov

61. Medical Subject Headings (MeSH)

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methylparaben

https://www.ncbi.nlm.nih.gov/mesh/67015358

MeSH Tree

http://www.nlm.nih.gov/mesh/meshhome.html

Preservatives, Pharmaceutical

https://www.ncbi.nlm.nih.gov/mesh/68011310

62. GHS Classification (UNECE)

GHS Classification Tree

http://www.unece.org/trans/danger/publi/ghs/ghs_welcome_e.html

63. EPA Substance Registry Services

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https://www.epa.gov/privacy/privacy-act-laws-policies-and-resources

EPA SRS List Classification

https://sor.epa.gov/sor_internet/registry/substreg/LandingPage.do

64. PATENTSCOPE (WIPO)

SID 403031139

https://pubchem.ncbi.nlm.nih.gov/substance/403031139